TIME DEPENDENT DIFFUSION KINETICS FOR AN ELECTRON BEAM INCIDENT IN WATER VAPOR

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to my parents, wife and daughter

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The problem of the time dependent effects, both transient and steady state, of diffusion kinetics on the spatial yields generated by a monoenergetic, collimated electron beam incident in water vapor is investigated for incident energies below 2 keV. Spatial yields of the primary species created by the electron energy degradation are based on spatial yield spectra generated by Daniel Rio in his Ph. D. thesis (1983). Diffusion is calculated in the spherical approximation.

It is observed that proton transfer from ions to H_2O and electron transfer to ions from H_2O, and proton hydration can be treated as globally instantaneous, while electron-proton recombination can be treated as locally instantaneous only, because of charge separation. Above 500 eV charge separation is fairly negligible, and the approximation of globally instantaneous recombination can be made. This approximation is also employed below 500 eV as a rough estimate, where charge separation becomes increasingly significant.

Diffusion kinetic results are calculated via a modification of the BOAT code of Dash and Pergament, which was designed to calculate turbulent jet entrainment with chemistry in rocket nozzle exhaust plumes. These results are explained in terms of diffusion modification of the corresponding pure kinetic system. Results fall into two regimes (early and late chemistry) depending on the ordering of kinetic onset time and diffusion convergence time. Dependence of trends on injection rate and medium density are identified. Results are critically compared with steady state results which incorporate the same inputs.

CHAPTER I
INTRODUCTION

Background and Motivation

The irradiation of gaseous and liquid media by either photons, protons or other positive ions ultimately involves the generation of electrons and their subsequent interaction with the medium. This interaction takes place within a time interval referred to as the 'physical' phase, involving excitation and ionization within 10^{-15} sec, and dissociation of molecules within 10^{-13} sec (Hart and Platzmann, 1961; Magee, 1963). In the case of liquid water, ion molecule reactions are pushed back into this time phase ($< 10^{-10}$ sec) by the factor of concentration. In the gaseous phase, this is not the case. This stage is followed by an intermediate stage known as the 'physico-chemical' phase, which primarily marks the end time of dissociation of molecules and the beginning of ion molecule reactions. Diffusion of the electron, i.e. the thermalized electron, begins at this time.

In the liquid case the 'chemical' phase starts around 10^{-10} -10^{-8} sec, at which time neutral reactions begin and molecular diffusion begins to have an effect. The events occurring in this phase have been treated by various researchers in terms of an assortment of different diffusion kinetic models. Most noteworthy has been the work of Kupperman (see Kupperman and Belford, 1962a, 1962b; Kupperman, 1974), Magee (1957) and Magee and Chatterjee (1978, 1980).

In order to model the 'chemical' phase behavior, however, physical inputs deriving from the earlier 'physical' phase are required. This

connection between the processes and events taking place in these two phases is generally known as the interface between radiation chemistry and radiation physics. The identification of the relevant early time events and the accurate calculation of their cross sections have been the object of intense effort--and the subject of vigorous debate--over the past several years among those involved in this effort (for example, see Douthat (1983), Inokuti, (1983)).

A significant contribution to this effort has been made by Green and coworkers at the University of Florida. With particular regard to the problem of electron degradation in water vapor are the works of Green et al. (1971), Olivero et al. (1972) and Kutcher and Green (1974a), the latter work extending to the case of liquid water. These inelastic cross sections, along with fits to elastic cross section data by Porter and Jump (1978) have been compiled and updated by Zaider, Brenner and Wilson (1982) at Los Alamos National Labs. On the basis of these cross sections it is now possible to calculate 'chemical' phase events on the basis of "first principles," rather than, as had previously been the case, by assuming resonable spatial distributions and working backwards from known experimental g-values (yields per 100 eV). In this regard, two widely divergent approaches have been taken in the calculation of these later time events. The Oak Ridge group (see Hamm et al., 1978; Hamm et al., 1983; Ritchie et al., 1978; Turner et al., 1980; Wright et al., 1983a and b) have constructed a Monte Carlo program which follows the electron into the chemical stage and actually calculates chemical reactions stochastically. Such an approach can probably be considered to be state of the art in simulation.

A different approach has been taken by Green and coworkers. This approach consists of following the electron in its degradation and multiple scattering during the physical phase, at which point a statistical profile of inelastic events is taken from which a smoothed mean spatial and spectral density of inelastic events is obtained. This spatial spectral density is called the spatial yield spectrum, (Jackman and Green, 1979), generalizing on the concept of the yield spectrum (Green, Garvey and Jackman, 1977), which is a modification of the concept of the degradation spectrum of Spencer and Fano (1954). It is a nearly universally invariant quantity for all gaseous media, possesses advantageous mixing and scaling properties, and from it the spatial yields of states, and from them the spatial yields of the various 'initial deposition' species follow in a simple manner.

Why the Continuous Electron Beam?

This thesis takes as its starting point the work of the previous thesis by Rio (1983) which calculates spatial yields for water vapor via the Monte Carlo technique alluded to, and inputs them into a time dependent diffusion kinetic calculation for continuous, steady electron beam turned on at $t = 0$.

Rio, in his thesis (1983), did attempt to calculate steady state diffusion kinetics of this system. However, at this point in time, these efforts remain incomplete--close to final answer but beset by questions of numerical technique and reproducibility. Results of this study will be of use in the resolution of this problem.

In previous and other current radiological work a short pulse electron beam rather than a continuous, steady beam is considered.

Kupperman and Belford (1962a, b), assuming low injection rates (also known as dose rates), and therefore isolated tracks, calculated for the case of an initial pulse, the effects of which die out after its passage through that spatial element of the medium. Magee and Chatterjee (1978), implementing the 'prescribed diffusion' model, account for dose rate dependence, that is to say, nonlinear effects due to the chemistry. They also calculate for an initial pulse. The present, ongoing Monte Carlo work of the Oak Ridge group (see previous section) also calculates for an initial pulse.

In the microscopic realm, the calculations carried out here for a continuous beam, may not be the most relevant configuration. However, for high enough dose rate so that track overlap is significant, this macroscopic approach, averaging out track structure, should be valid. In the microscopic realm, it may also apply.

Outline of Thesis

In Chapter II we begin by identifying the spatial yields. As is noted there, it was decided to redo the work of fitting the spatial yield spectra. It is found that the spread in the spatial fall off rate over spectral energy of the electron (involved in the event counted) can be adequately represented by a span between its two extreme spectral limits. The g-values for various states, and, summing over branching ratios devised by Rio, for the various primary species, can then be divided into a low and high spectral component. It is found that this high spectral component contributes proportionately less and less at higher incident energy, and that, as a result, there is a decrease in charge separation at higher incident energy.

The exponential fall off seen by Rio in the data out to two to three decades is confirmed. The data are presented graphically so that there can be no mistaking what their trends are--to within the noise limit of the Monte Carlo data. It is found that for incident energy around or below 1 keV, the contours are sufficiently close to spherical that the spherical approximation is adequate. This is discussed further in Appendix D, where steady state axisymmetric diffusion is calculated.

In Chapter III we review some basic mathematical results for pure kinetics and pure diffusion. Of specific interest: dependence of reaction time on source strength, reaction rate coefficient, and medium density, and dependence of diffusion convergence time on medium density. We then address diffusion kinetics of two body decay. First we calculate the simplest case, namely that of one species on itself. We follow this up with the case of that between two distinct species. In the two species case, the specific reaction, $H + OH + M \rightarrow H_2O + M$, in the context of the radiological deposition is used.

The two species diffusion kinetic problem for the particular reaction, $H + OH + M \rightarrow H_2O + M$, is considered at the intermediate density of the three medium densities considered in Chapter VI, at all three injection rates. In this way its effect can be isolated. We find that the resultant trends can be explained in terms of (1) the ordering of reaction time and diffusion convergence time, (2) majority and minority reactants (per source term), and (3) relative diffusion coefficients.

At this point the time dependent diffusion kinetic code written for the purpose of this thesis, DIFKIN, is brought into play. This code is discussed in complete detail in Appendices A and B. In effect, Appendices A and B are a user's guide.

In Chapter IV the ion reactions are considered. From a simple argument we identify the concentrations of neutral species subsequent to local electron-proton recombination. Noting the decrease in change separation at higher incident energy, it follows that at higher incident energy, the approximation of global recombination becomes valid. The possibility of upgrading the code to take into account charge separation exists, and should prove to be a very interesting direction in which to take this work.

This chapter is closed out with a calculation of dependence of the time scales of the ion reactions on medium density and injection rate, based on results of Chapter III. This calculation is based on a simple but accurate simplification of the ion reaction set (10 reactions) into two reactions.

In Chapter V we consider the pure kinetics of the neutral reaction set. Trends in medium density and injection rate are identified. Principal pathways and their trends in medium density and injection rate are identified and displayed. It is found that above a minimum injection rate qualitative dependence on injection rate disappears. The question of stiffness of the system of kinetic equations is addressed.

The kinetic systems considered are those which obtain at the center of the plume for the representative incident energy, 1 keV, ignoring diffusion. It serves the purpose of a base for comparison so that the diffusion effect upon kinetics can be isolated.

This finally leads us to Chapter VI where we address the full diffusion kinetic system. We first consider the trends in medium density and injection rate at the chosen representative medium range incident energy, 1 keV. Specifically, three densities are calculated for: $6x10^{15}$ #/cc, $1.84x10^{19}$ #/cc (1 atm at 400 K), and $3.34x10^{22}$ #/cc (liquid density). The first two cases are calculated for T = 400 K, the last one for T = 300 K.

This choice is made for the sake of physical realism. All kinetic runs in Chapter V but one are also made at T = 400 K. A corresponding run is made at 300 K for the liquid density case to test for temperature sensitivity, and to provide a corresponding basis for comparison between kinetic and diffusion kinetic results at this density.

At each of these densities the trend in injection rate is observed by calculating for three values (exception: two, in the case of the low pressure vapor) corresponding to late chemistry, borderline chemistry, and early chemistry.

Finally, in Chapter VII, the results obtained here are compared with results of Rio, Dayashankar, Schippnick, and Green (unpublished work) for the steady state case. Future directions for this work are discussed. Experimental set-ups in which these results may be tested are discussed, especially in the context of current radiation chemistry research, in particular, the Febetron work of Hanrahan and coworkers (this campus).

CHAPTER II
SPATIAL YIELDS

In previous work in radiation chemistry predicated upon a macroscopic diffusion kinetic model (Kupperman and Belford, 1961a, 1962b; Magee and Chatterjee, 1978, 1980), the "initial" spatial yields have in general been estimated on the basis of known experimental g-values (yields per 100 eV), assuming a reasonable spatial dependence. Calculation of these initial spatial yields from first principles requires (1) a comprehensive compilation of collision cross sections, and (2) solution of the transport equation to which these cross sections are inputs.

A significant contribution to this first task has been made over the past several years by the research group led by Alex Green at the University of Florida. Of particular interest to the problem of electron degradation in water vapor are the work of Green et al. (1971), Olivero et al. (1972) and Kutcher and Green (1976a), the latter work extending to the case of liquid water. These cross sections, along with fits to elastic cross section data by Porter and Jump (1978) have recently been compiled and updated by Zaider, Brenner and Wilson (1983) at Los Alamos National Labs.

In his Ph. D. thesis (1983) Daniel Rio has recently calculated these initial spatial yields by means of a Monte Carlo technique developed in this group (Jackman, 1978; Kutcher and Green, 1976b). In this calculation the primary electron and any secondaries which it may have created are degraded randomly according to probabilities determined

by the set of collision cross sections inputted into the code. The collisional history raw data are not used to directly calculate the spatial yields. Instead, the spatial yield spectra approach of Green et al. (Jackman and Green, 1979; Green and Singhal, 1979) is employed.

This approach is based upon the calculation of a quantity, $U(E,\rho,z,E_o)$, called the spatial yield spectrum, or four dimensional yield spectrum, which is a function of incident energy, E_o, spectral energy, E, and cylindrical spatial coordinates, ρ and z. It is defined by

$$U(E,\rho,z,E_o) = N(E,\rho,z,E_o)/\Delta\tau \tag{2.1}$$

where $N(E,\rho,z,E_o)$ is the number of inelastic events taking place per unit time, normalized to injection rate, with spectral energy in the interval ΔE centered at E, in the volume element $\Delta\tau = 2\pi\rho d\rho dz$ centered at (ρ,z). Like the two dimensional yield spectrum (Green, Garvey and Jackman, 1977) which it reduces to,

$$U(E,E_o) = U_a(E,E_o)\theta(E_o-E_m-E) + \delta(E_o-E) \tag{2.2}$$

the four dimensional yield spectrum is divided into a continuous spectrum extending from E_m up to $E_o - E_m$, $U_a(E,\rho,z,E_o)$, and the contribution of the undegraded electrons, called the source term, $D(\rho,z,E_o)$ (Green and Singhal, 1979):

$$U(E,\rho,z,E_o) = U_a(E,\rho,z,E_o)\theta(E_o-E_m-E) + D(\rho,z,E_o)\delta(E_o-E) \tag{2.3}$$

where E_m is the threshold of inelastic events, $\theta(E)$ is the Heaviside step function and $\delta(E)$ is the Dirac delta function.

Defining $p_i(E)$ as the probability of exciting the i-th inelastic state, given an inelastic event, the spatial yield for this state, $J_i(\rho,z,E_o)$, is given by

$$J_i(\rho,z,E_o) = \int_{E_i}^{E_o} p_i(E')U(E',\rho,z,E_o)dE' \qquad (2.4)$$

where E_i is the i-th threshold energy. The probability $p_i(E)$, is given by $\sigma_i(E)/\sigma_{inel}(E)$. The spatial yield spectrum is therefore seen to unite into one function, in effect a source function, the common, shared spectral and spatial information of all inelastic events.

Finally, summing over the appropriate states weighted by the appropriate branching ratios, one obtains the spatial yields of the "primary yield" species produced by the degradation of the incident electrons (primary electrons) and secondaries and tertiaries (higher generations are negligible). For water vapor these species are H, OH, H_2, O, H_2O^+, H^+, OH^+ and the thermal electron. O^+ production (less than 1%) is negligible.

The Deposition Spectrum

Singhal et al. (1983), in their work on electron energy degradation in neon, define a quantity which they call the deposition spectrum. As the electron falls below threshold it is counted in the spectral and spatial bins in which it falls, and its subsequent elastic degradation

is not followed. Since the threshold of inelastic events in neon is fairly high (16.7 eV), there is room in this interval for spectral structure.

The low inelastic threshold of water (threshold of rotational and vibrational states is .12 eV precludes this, although, if one wanted to, one could keep track of the spectral structure below the threshold of electronic excitations (7.6 eV). Thus, in the case of water vapor, it suffices to count in one bin below threshold, which is what Rio (1983) has done.

Thus, apart from a normalization constant, this deposition spectrum for the case of water vapor, somewhat in the manner of the source term at the other end of the spectral scale, is merely a scaled spatial density--its spectral aspect reduces to a mere formality. In fact Rio defines the deposition spectrum for H_2O, $DS(\rho,z,E_o)$, as the spatial density of subthreshold electrons. It therefore integrates out to $N(E_o)$, the electron yield due to ionization in addition to the initial or injected electrons (primaries).

The motivation for keeping separate count of these events was to identify the spatial yield of the thermal electrons, i.e., those electrons which have fallen below threshold (at 300 K, the thermal energy of the electron is about .03 eV). However, as we shall see below, this was not really necessary. At these low energies, the electron has essentially stopped moving, and its spatial distribution, to within a normalization factor, has converged. Thus, to within a normalization factor, the deposition spectrum in the case of water vapor is identical with the low spectral end of the spatial yield spectrum.

Analytic Representation

Green and Singhal (1979) represented the two dimensional yield spectra calculated by Green, Garvey and Jackman (1977) and Green, Jackman and Garvey (1977) by the following common form:

$$U(E,E_o) = C_o + C_1X + C_2X^2 \tag{2.5}$$

where $X = X(E,E_o) = E_k^{\Omega}/(E + L)$ with E_o and E measured in eV, and $E_k = E_o/1000$. They found that they could simultaneously fit yield spectra for a variety of gases with Ω set to .585 and L = 1 eV.

The first term, which is in general a small constant value, serves to represent the small limiting value at high spectral energy which is essentially independent of incident energy. The second and third term together represent the increasing value of the yield spectra with decreasing spectral energy.

In subsequent work Singhal and Green (1981) and Singhal et al. (1983) fit the spatial yield spectra of O and Ne with the following generalization of the two dimensional form devised by Green and Singhal (1979), called the microplume model:

$$U_a(E,\rho,z,E_o) = \sum_{i=0}^{3} C_iX^i \frac{A_i(E_o)}{R^3} G_i(\rho,z,E_o) \tag{2.6}$$

$$D(\rho,z,E_o) = \frac{A_s(E_o)}{R^3} G_s(\rho,z,E_o) \tag{2.7}$$

where

$$G_i(\rho,z,E_o) = \exp[-(\frac{\alpha_i r}{1+\delta_i z} + \beta_i{}^2 z^2 - \gamma_i z)] \tag{2.8}$$

and the coefficients $A_i(E_o)$ are normalization factors for the spatial integrals of the $G_i(\rho,z,E_o)$. The quantity $R(E_o)$ is the range in units of gm/cm^2. The spatial yield spectrum is in units of $\#/eV/(gm/cm^2)^3$. The spatial coordinates are in units of $R(E_o)$. The quantities G_i (and therefore A_i) were defined in a piecewise fashion for the forward and backward plumes, i.e. for $z > 0$ and $z < 0$. Although this was done for the sake of computational convenience, and allowed for the easy calculation of forward and backward spatial integrals, it results in an unphysical discontinuity in the spatial contours at the $z = 0$ plane.

Rio (1983) observed that the data exhibited essentially exponential falloff in all directions outward from the forward peak, and elliptical contours centered about the peak. He devised the following continuous form to represent these features:

$$G_i(\rho,z,E_o) = \exp(-\beta_i d\sqrt{\rho^2 + \delta^2(z-z_o)^2}) \tag{2.9}$$

where d is medium density in gm/cc and ρ and z are in units of cm. As it stands, this form contains one mistake, but a reparable one: z_o, which is presented as independent of d, should be set inversely proportional to d. The Rio form is therefore correctly stated by

$$G_i(\rho,z,E_o) = \exp(-\beta_i\sqrt{\rho'^2 + \delta^2(z'-z_o')^2}) \tag{2.10}$$

where $\rho' = \rho d$ and $z' = zd$ and z_o' is in units of gm/cm^2. Knowing the densities at which the various runs were made, the correction follows immediately.

It was the original intention of this thesis to use Rio's fits as inputs. However, other mistakes have been made in this work, and for this reason the author decided to refit these data. At the instigation of Professor Green, a group effort was then undertaken to produce data at higher energies and one lower energy in order to exhibit trends in incident energy more clearly. The availability of these extensions to the data base was extremely helpful. The author is especially grateful to Dr. Dayashankar and Mr. Jerome Schwartz for their work in the generation of these data sets.

The Yield Spectrum

The two dimensional spectra, as Green, Garvey and Jackman (1977) observed, possess a fairly characteristic pattern as a family of curves when plotted against E, namely, a fall off from a flat initial level, scaled very nearly by E_o, which falls roughly as between the inverse first and second power in E, to a constant level independent of E at the upper spectral end. The flat initial level reflects the drop off of the total inelastic cross section with decreasing energy below its peak. As previously noted, this behavior was represented by Green and Singhal (1979) by the form given in Eq. (2.1).

If the yield spectra are calculated down below the threshold of electronic excitations into the vibrational and rotational spectrum, a rather predictable bookkeeping result follows. Because these processes can degrade the electron's energy only in small amounts, the frequency of inelastic events increases as the electron degrades through this region, and, correspondingly, the yield spectra start to increase steeply with decreasing E in this region.

However, the details of the yield spectrum in this low range are of no significance to the main purpose of the yield spectrum, which is the calculation of spatial species yields. These low lying vibrational and rotational states do not contribute. We therefore limit our attention to spectral energies above .5 eV.

The original form of Green and Singhal is found to well represent the two dimensional yield spectrum at all interesting spectral energies. In fact, it can even be simplified without loss of accuracy if the form $X = E_k^{\Omega}/(E + L)$ is replaced by the form $X = E_k^{\Omega}/\sqrt{E^2 + L^2}$, and Ω is fixed at .5 rather than .585, and L is allowed to vary. C_1 can then be set to zero, and we obtain $C_o = .0282$, $C_2 = 902.$, and $L = 3.21$ eV. In effect, the middle plume is dispensed with. The two dimensional yield spectrum and the fit to it are graphed in Fig. 2.1. This work involved some collaboration with Professor Green and Dr. Dayashankar.

The Spatial Yield Spectrum

Presentation and characterization of data. In considering the spatial yield spectral data, since the two dimensional spectrum has already been tied down, it is natural to normalize it out, so that the remaining spectral dependence stands out as a separate entity. We therefore define normalized spatial yield spectra and normalized deposition spectra:

$$U_n(E,\rho,z,E_o) = U_a(E,\rho,z,E_o)/U_a(E,E_o) \qquad (2.11)$$

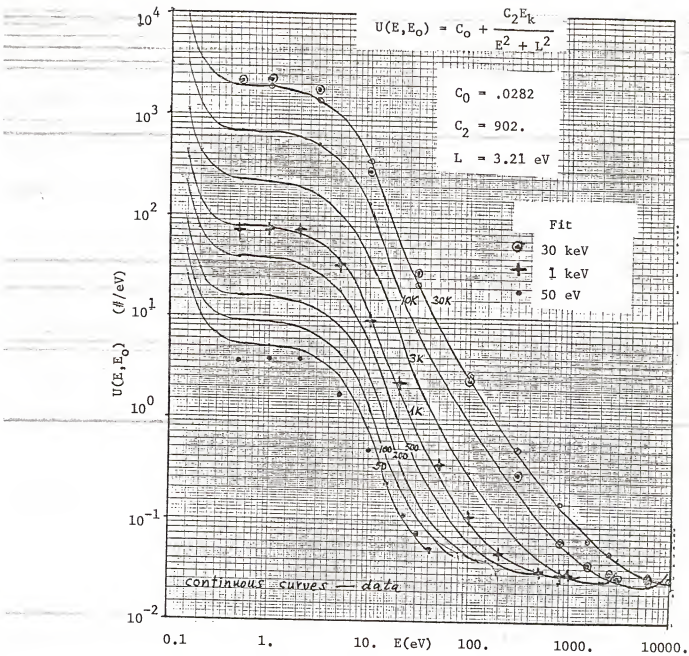


Figure 2.1. Two dimensional yield spectra, $U(E,E_o)$ vs. E. Data and fit.

$$DS_n(\rho,z,E_o) = DS(\rho,z,E_o)/N(E_o). \tag{2.12}$$

The source term is already normalized (see Eq. (2.7)).

It may seem strange to speak of "normalized spectra" in that what has been normalized out of them is exactly what makes them spectra, i.e., namely, that they should reduce to spectra upon spatial integration. What they are, really, is spectrally parametrized families of spatial densities. However, the term "normalized spectra", even though it is somewhat anomolous, is convenient.

In order to accurately characterize these data, graphs of ρ and z profiles were plotted for all incident energies at which data existed. Contour plots were then inferred from these profiles for representative cases. Representative profiles of the raw data at E_o = 100 eV, 1 keV and 10 keV are shown in Figs. 2.2-2.4 for the normalized deposition spectra and source term, and in Figs. 2.5-2.7 for the normalized spatial yield spectra. Smoothed contour plots are also shown for the normalized spatial yield spectra at those same energies in Figs. 2.8-2.10.

From these profiles and contour plots we observe the following trend in E_o: for low E_o the pattern of contours is concentric elliptical; at intermediate E_o, the pattern becomes singly confocal; while for $E_o \gtrsim 10$ keV there has evolved a highly prolate singly confocal 'core' surrounded by a more rounded 'penumbra'.

Turning our attention next to the 100 eV profiles, we note that the source term presents a much steeper falloff than does the more relaxed deposition spectrum (note: the source term is only noticeable at and below 500 eV, no data exist for it above 1 keV for the number of primary

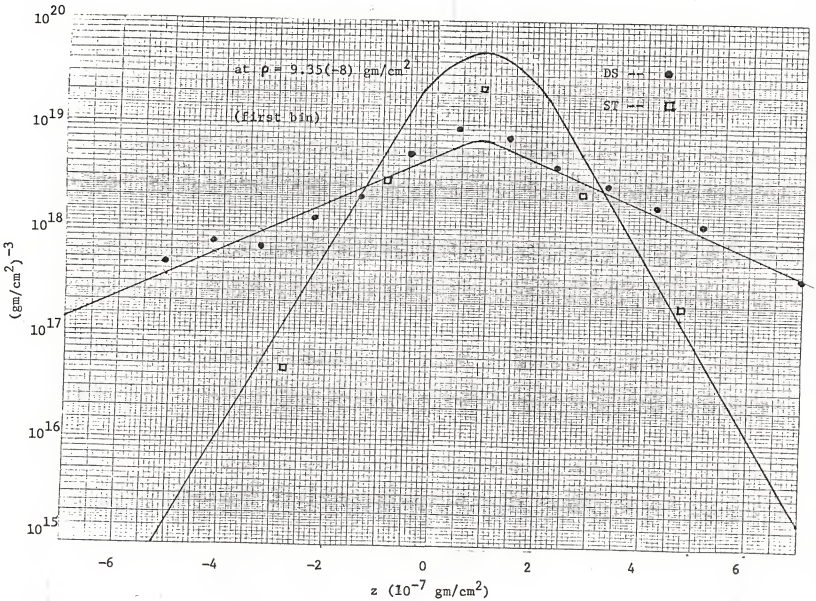


Figure 2.2. Normalized deposition spectrum ( ) and source term ( ). E_o = 100 eV. Data and fit.

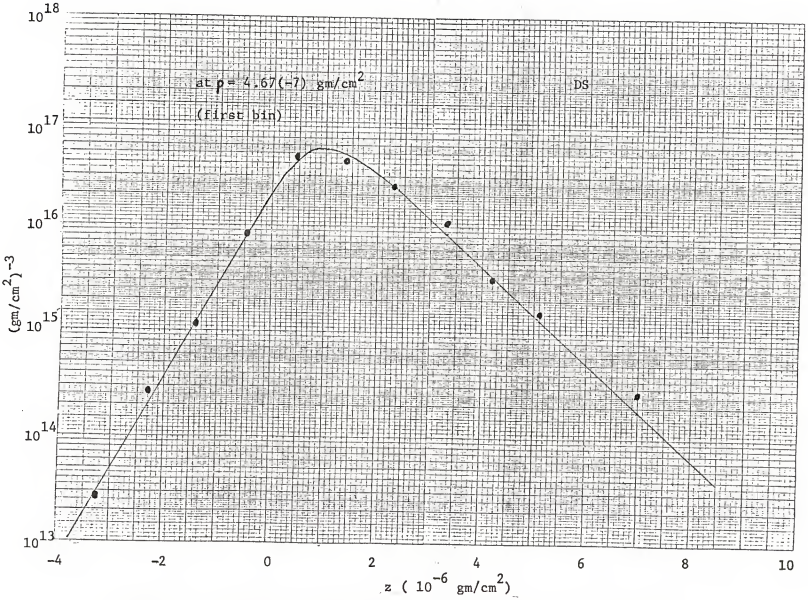


Figure 2.3. Normalized deposition spectrum E_o = 1 keV. Data and fit.

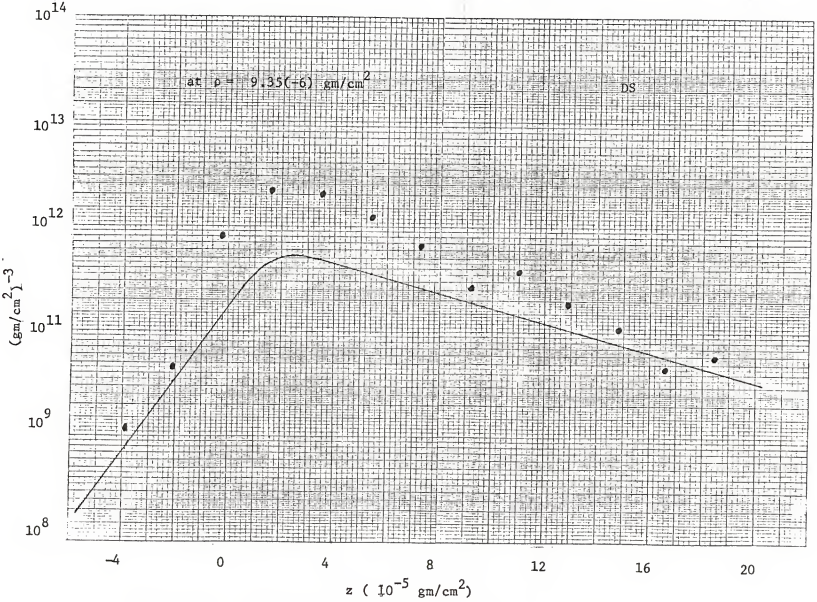


Figure 2.4. Normalized deposition spectrum. E_o = 10 keV. Data and fit.

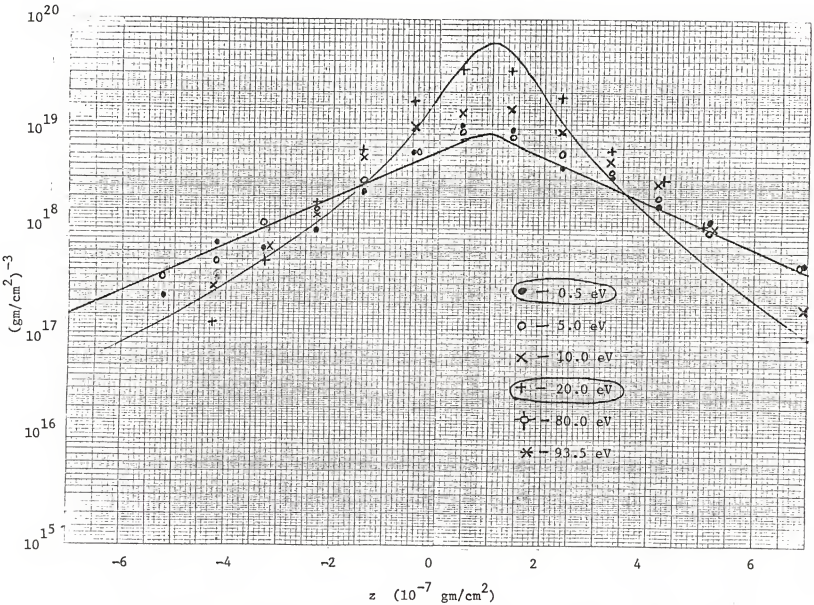


Figure 2.5. Normalized spatial yield spectrum. E_o = 100 eV. Data and fit.

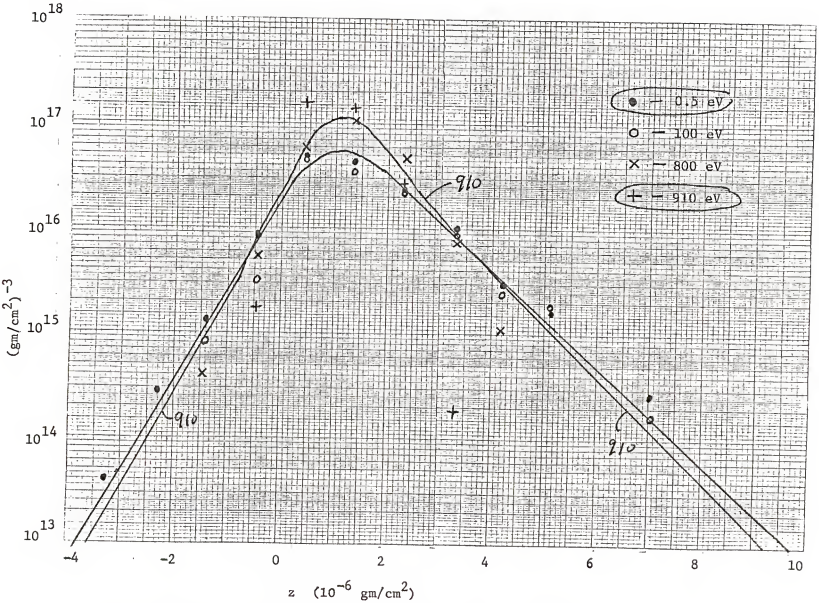


Figure 2.6. Normalized spatial yield spectrum. E_o = 100 keV. Data and fit.

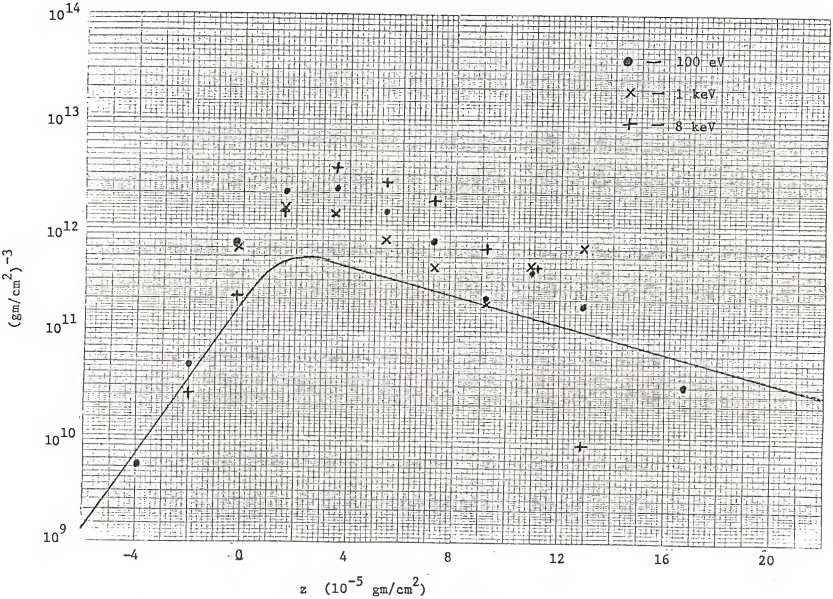


Figure 2.7. Normalized spatial yield spectrum. E_0 = 10 keV. Data and fit.

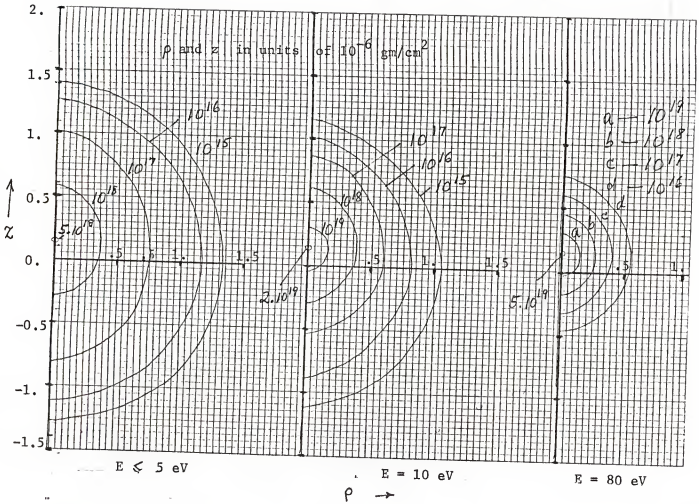


Figure 2.8. Smoothed contours of raw data of the normalized spatial yield spectrum for $E \leq 5$ eV, $E = 10$ eV, and $E = 80$ eV. $E_o = 100$ eV.

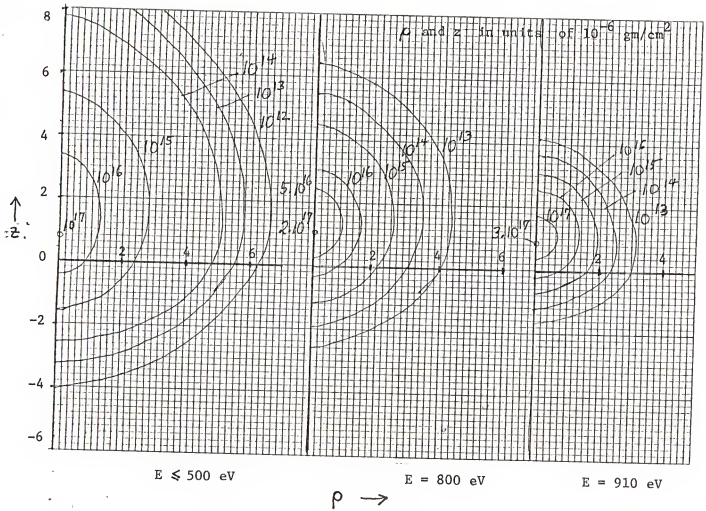


Figure 2.9. Smoothed contours of raw data of the normalized spatial yield spectrum for E = 500 eV, E = 800 eV, and E = 910 eV. E_o = 1 keV.

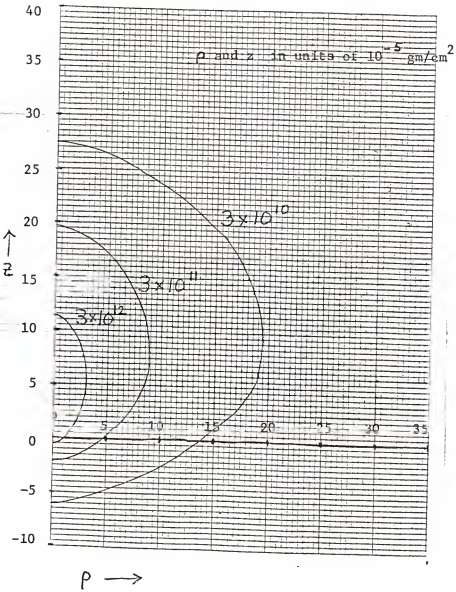


Figure 2.10. Smoothed contours of raw data of the normalized spatial yield spectrum for $E \leq 8$ keV. $E_o = 10$ keV. Pattern is essentially converged.

histories implemented in the generation of our data sets). We note that its peak is essentially aligned with that of the deposition spectrum.

Comparing now the profiles of the normalized spatial yield spectra, it becomes clear that they lie in between the limits of the normalized deposition spectra and the source term. Contour peaks are all seen to be aligned. Spectral dependence of contour shape is seen to be none at 100 eV, slight at 1 keV and at 10 keV. Fall off rate decreases monotonically from a maximum value at the source term, and the contours, in general, are seen to converge to the contours of the normalized deposition spectrum by roughly 10 eV for E_o = 100 eV, by roughly 500 eV for E_o = 1 keV and by roughly 8 keV for E_o = 10 keV.

Theoretical aside. That they should do so is predicted by continuous slowing down theory. The stopping power in the Born limit, $dE/dx \propto \ln E/E \propto E^{-3/4}$ (Bethe, 1932). The distance traveled up to degradation of the electron's energy down to E, which we may denote as $r(E,E_o)$, is given by

$$r(E,E_o) = \int_E^{E_o} \frac{dE}{-dE/dx} \tag{2.13}$$

From this it follows that the ratio $r(E,E_o)/r(0,E_o)$ is given by

$$r(E,E_o)/r(0,E_o) = 1 - (E/E_o)^{7/4} \tag{2.14}$$

from which it follows that dr/dE falls to zero as E approaches zero. The quantity $r(0,E_o)$ is defined as the range or effective range and symbolized, $R(E_o)$.

The above derivation is valid if E_o is well enough above the Born limit. For incident energies in the low end of the Born limit and below (typically $E_o \lesssim 200$ eV) the correction to the stopping power based on corresponding correction to cross sections it is based on, given by Green and Barth (1965) and further developed by Stolarski and Green (1967) must be taken into account.

Specifically, the stopping power mimics the cross sections of which it is a weighted sum, and turns around and drops to zero as the electron energy drops to threshold. As a result, the energy at which the electron has converged in its motion is a smaller fraction of incident energy at lower incident energy, until at the very lowest incident energies the convergence has disappeared. This relative falling back of the range convergence energy with decreasing incident energy is shown in Fig. 2.11, where $r(E,E_o)$, inferred from these spatial yield spectral data by means of continuous slowing down theory, is plotted. This point is discussed in greater detail below.

Analytic representation. Three basic features of the contours at a given spectral energy, E, can be identified: fall off rate (in essence, range), offset, and shape. In the interest of simplicity, the more differentiated shape of the contours at higher incident energy will not be addressed, and only an average fit will be attempted there. The following form is chosen to represent the evolution of shapes just described, closely at low and medium incident energies, and in an average way at high incident energy:

$$G(\rho,z,E_o) = \exp\left[-\beta\left(\sqrt{\gamma^2\rho'^2 + (z' - z_o')^2} - \varepsilon(z' - z_o')\right)\right] \qquad (2.15)$$

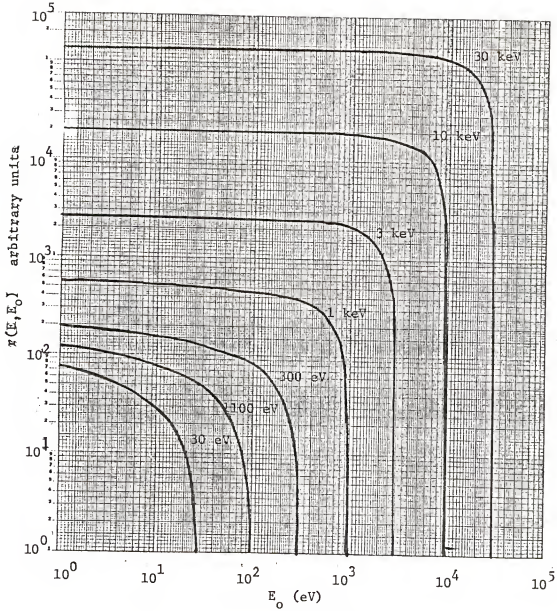


Figure 2.11

Figure 2.11. $r(E,E_o)$ vs. E for representative sequence of values of E_o. Inferred from $\beta(E_o)$ via CSDA.

for which the normalization factor, $A_I(E_o)$, is given by

$$A(E_o) = (1-\varepsilon^2)^2\gamma^2\beta^3/8\pi \tag{2.16}$$

This form may be described as affine singly confocal. At low energy, ε is kept equal to zero, with $\gamma > 1$, yielding concentric prolate elliptical contours. In the transition range γ decreases towards 1 as ε takes over. At higher energies ε continues to increase, but γ decreases below 1 in order to represent in an average sense the rounded penumbra.

The true eccentricity of the elliptical contours is given not by ε, but by $\varepsilon_{tr} = \sqrt{1 - (1-\varepsilon^2)/\gamma^2}$. On the basis of the stochastic data obtained so far, there is no definitive indication of a trend toward oblateness. We, therefore, constrain ε_{tr} to fall back to zero as E_o increases. In this way the roundedness of the penumbra is represented at the expense of the prolateness of the inner core.

The results of fitting the parameters β, z_o', ε and γ to the deposition spectra energy by energy are presented in Figs. 2.12-15. The following forms were found to adequately represent these trends, taking into account the above-mentioned nonperturbative constraint on γ:

$$\beta(E_o) = \frac{a}{1+bE_o^{\,p}} \tag{2.17}$$

$$z_o'(E_o) = c_1E_o^{\,q_1} + c_2E_o^{\,q_2} \tag{2.18}$$

$$\varepsilon(E_o) = \left[\frac{P\ \ln(E_o/E_\varepsilon+1)}{P\ \ln(E_o/E_\varepsilon+1) + 1}\right]^Q \tag{2.19}$$

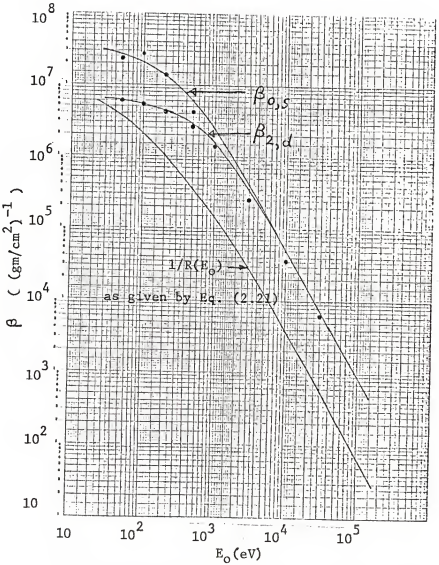


Figure 2.12. $\beta(E_o)$ vs. E_o and $\beta_{o,s}(E_o)$ vs. E_o. Also graphed is $1/R(E_o)$ from Eq. 2.21. Values obtained from fitting spectral data at individual E_o values, and regression.

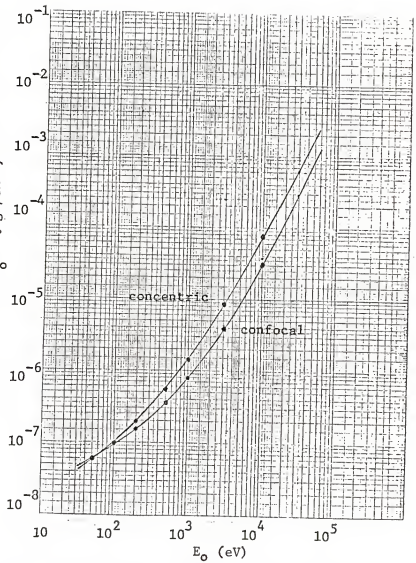


Figure 2.13. $z_o'(E_o)$ vs. E_o. Both confocal and concentric fits. Values obtained from fitting spectral data at individual E_o values, and regression.

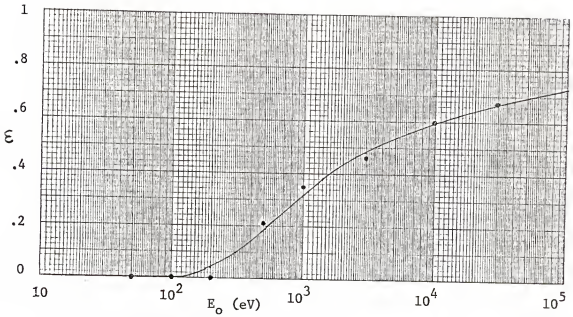


Figure 2.14. $\varepsilon(E_o)$ vs. E_o. Values obtained from fitting spectral data at individual E_o values, and regression.

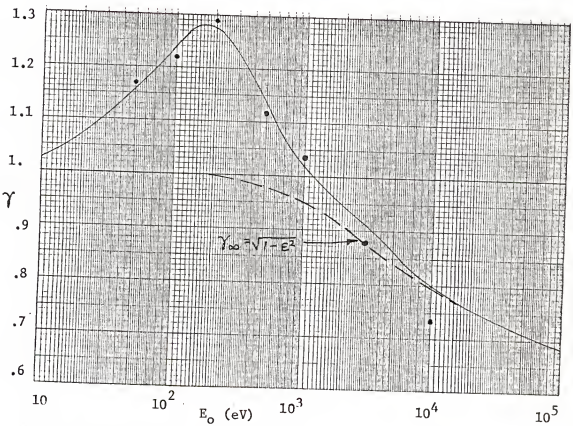


Figure 2.15. $\gamma(E_o)$ vs. E_o. Values obtained from fitting spectral data at individual E_o values, and regression.

$$\gamma(E_o) = \left[1 + \alpha(E_o/E_\gamma)e^{-E_o/E_\gamma}\right]\left[(1-\gamma_\infty)\frac{\sigma + 1}{\sigma + e^{E_o/E_\sigma}} + \gamma_\infty\right] \tag{2.20}$$

$$(\text{where} \quad \gamma_\infty = \sqrt{1 - \varepsilon^2(E_o)})$$

where the energy dependence fitting parameters are given in Table 2.1. The quality of fit is indicated in Figs. 2.2–4 where the graphs of the fit have been overlaid on the data.

The form $\beta(E_o)$ is identical to the form of the inverse range in Singhal and Green (1981). We can compare our results with Singhal and Green, and with experimental data of electron penetration of arbitrary media of Katz and Penfold (1952). These data and more recent data have been fitted by Green (private communication, 1984) by the formula,

$$R(E_o) = \left(\frac{E_k}{1157}\right)^{7/4}\left(1 + \frac{.525}{E_k}\right) \tag{2.21}$$

where $E_k = E_o/1000$. The corresponding inverse range is plotted along with $\beta(E_o)$ in Fig. 2.12. It is to be noted that the accuracy of the form of Eq. (2.21) is less at lower energies. The agreement in proportionality of the two quantities is very good, with a factor of proportionality of about 10. For exponential fall off this implies setting the range at the distance at which the spatial integral has included 99.5% of the total. This is a little further out than the usual definition of range (see Green, 1955) but about right.

The fit to $\beta(E_o)$ can be improved a little by going over to the form

$$\beta(E_o) = \frac{a}{E_o^{\varepsilon} + bE_o^{p}} \tag{2.22}$$

TABLE 2.1
Fitting Parameters for Spatial Yield Spectra

$\beta(E_o)$ and $\beta_{o,s}(E_o)$:

a = 5.46(6),	b = 2.65(-5),	p = 1.66,		Eq. (2.17)
a = 1.34(7),	b = 2.65(-5),	p = 1.75,	ε = .197	Eq. (2.18)
k = 4.56				

$z'_o(E_o)$:

confocal	concentric
c_1 = 7.29(-9)	c_1 = 4.05(-9)
c_2 = 1.11(-12)	c_2 = 2.41(-12)
q_1 = 0.543	q_1 = 0.662
q_2 = 1.88	q_2 = 1.88

$\varepsilon(E_o)$:

E_ε = 251.
P = 48.2
Q = 90.6

$\gamma(E_o)$:

α = 0.751
E_γ = 185.
E_σ = 407.
σ = 736.

where $p = 1.75$ and ε is a small value. Specific values of a, b and ε are given in Table 2.1. This form is preferable to the form of Eq. (2.17) because it satisfies a requirement of continuous slowing down theory (it should be noted that Eq. 2.21 also satisfies this requirement) - namely, that $R(E_o) \downarrow 0$ as $E_o \downarrow 0$ (threshold idealized).

A further requirement arises from the previously noted correction to the energy loss function (-dE/dx) below the Born limit which states that -dE/dx turns around and fall to zero as E_o decreases. Noting that

$$-\frac{1}{\frac{dE}{dx}(\varepsilon)} = R'(\varepsilon) \tag{2.23}$$

(this result follows from Eq. (2.13) and the definition of $R(\cdot)$ via the Fundamental Theorem of Calculus), it follows that $R'(E_o)$ must turn around and rise toward infinity as E_o decreases below the Born limit. The form of Eq. (2.22) does satisfy this requirement, and for this reason it is superior to the form of Eq. (2.17) for extrapolation to lower incident energies. It is on the basis of this form and Eq. (2.23) that the empirically inferred values of $r(E,E_o)$ plotted in Fig. 2.11 were obtained.

The E_o dependence of z_o' is shown to be approximately proportional to the range, as expected. The concentric z_o' starts to increase away from the true z_o' above 300 eV to compensate, as one would expect.

Since the primary reason for interest in the spatial yield spectra for the purpose of this thesis is to use them to obtain spatial yields for diffusion kinetics, we have also fit the spatial yield spectra with ε fixed at 0, i. e. using the concentric form, in order to make it easy to sphericalize them in order to use them as inputs in the

diffusion kinetic calculations carried out in this work which are based upon spherical geometry. Such fits will be somewhat poorer for higher incident energies, because of the inaccuracy introduced in the location of the offset. However, because of the averaging and spreading effect of diffusion, this is not a serious detraction. The full benefit of the greater realism of the confocal form, or of a yet more apt form, can find application as input to a general two dimensional diffusion kinetic code, such as the steady state code, DIFKT, written by Rio (Ph.D. thesis, 1983).

It next remains to fit the source term and the normalized spatial yield spectra. All that remains then is to identify the tighter fall off rate for the source term and the spectral dependence of the fall off rate over the spectral range of the normalized spatial yield spectra. The simplest approach would be to represent the spatial yield spectra by one plume with $\beta(E_o)$ replaced by $\beta(E_o,E)$, and, correspondingly, $A(E_o)$ replaced by $A(E_o,E)$. However, this disallows a simple procedure for the evaluation of the spatial yields via Eq. (2.4) in which the spectral energy dependence has been separated out.

In order to maintain this advantage devised by Green and Singhal (1979), we gate between spectral limits instead outside the exponential. Thus we set

$$U_n(E,\rho,z,E_o) = f(E,E_o)A_o(E_o)G_o(\rho,z,E_o) + (1-f(E,E_o))A_2(E_o)G_2(\rho,z,E_o). \tag{2.24}$$

The form of $f(E,E_o)$ implied by the Green-Singhal form is

$$f(E,E_o) = \frac{C_o}{C_o + C_2X^2} = \frac{C_o(E^2 + L^2)}{C_o(E^2 + L^2) + C_2E_o/1000} \tag{2.25}$$

Contiuous slowing down theory suggests a gate of the form

$$f(E,E_o) = 1 - r(E,E_o)/R(E_o)$$

$$= \frac{E^{\varepsilon} + bE^p}{E_o^{\ \varepsilon} + bE^p} . \tag{2.26}$$

We may adjust all three parameters ε, b and p to optimize the fit. We now have two candidate spectral gate forms.

It remains also to identify $\beta_o(E_o)$, $\beta_2(E_o)$ and $\beta_s(E_o)$. We may at once set $\beta_2(E_o) = \beta(E_o)$. Correspondingly we may set $\beta_o(E_o) = \beta_s(E_o)$. For the sake of clarity, the notation $\beta(E_o)$ will be replaced by the notation $\beta_d(E_o)$. It remains, therefore, to determine $\beta_s(E_o)$ and $f(E,E_o)$. (It also remains to be determined whether the form of Eq. (2.24) or the intra-exponential gate form

$$U_n(E,r,z_o,E_o) = A(E_o,E)G(\rho,z,E_o,E) \tag{2.27}$$

where

$$\beta = \beta(E_o,E) = f(E,E_o)\beta_s(E_o) + (1 - f(E,E_o))\beta_d(E_o) \tag{2.28}$$

more faithfully represents the data.

Fitting the source term data (spectral gate independent) and the spectral data for $\beta_s(E_o)$, we find that we obtain good fit, using the empirical form

$$\beta_s(E_o) = \frac{ka}{E_o^{\ \varepsilon} + kbE_o^{\ p}} \tag{2.29}$$

with k = 4.56. Thus, the faster fall off of the high spectral plume becomes progressively relatively less so with increasing E_o.

Fixing k, and varying the adjustable parameters of the CSDA suggested gate, we obtain a sevenfold decrease in χ^2 with the new values, $\varepsilon' = .674$, $b' = 2.99\ (-10)$, and $p' = 3.91$. This value of the χ^2 is essentially identical to that obtaining for the Green-Singhal gate!

This work suggests that there must be something very right about this empirical form! This comes as something of a surprise, and makes this pursuit more interesting.

An idea of the quality of fits can be gotten from viewing Figs. 2.16-18 where contours of fits have been plotted for representative spectral plumes - unfortunately, for the unadjusted parameters in Eq. (2.29) and for the wrong k, (k = 3.6), and comparing with the smoothed contours of the raw data in Figs. 2.5-7.

It might be commented that the ideal manner in which to proceed with this work is to display the spectral plume data in interval contour plots, and so that a precise idea of the shape of the spectral gate can be obtained.

Spatial Yields

Spatial yields for the various excited states (which either dissociate, ionize, or dissociate and ionize) and ionization states created by the electron's energy deposition are calculated via Eq.

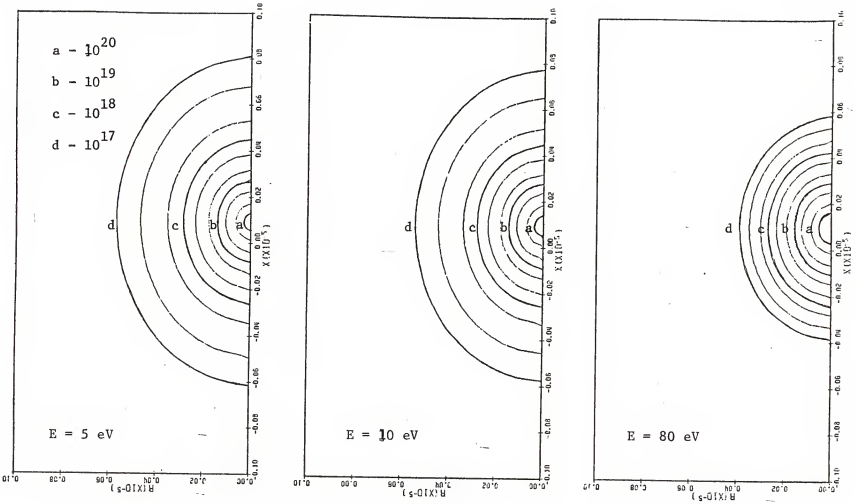


Figure 2.16. Contours of fit to normalized spatial yield spectrum for E = 5 eV, E = 10 eV, and E = 80 eV. E_o = 100 eV.

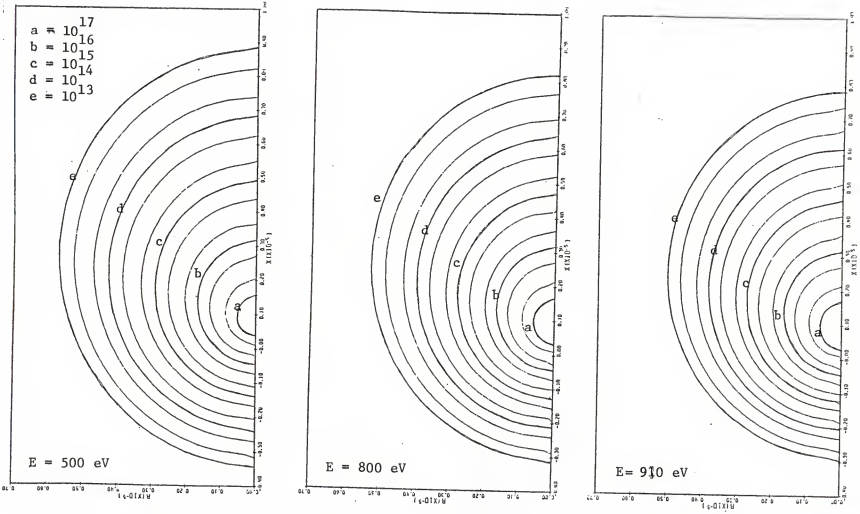


Figure 2.17. Contours of fit to normalized spatial yield spectrum for E = 500 eV, E = 800 eV, and E = 910 eV. E_o = 1 keV.

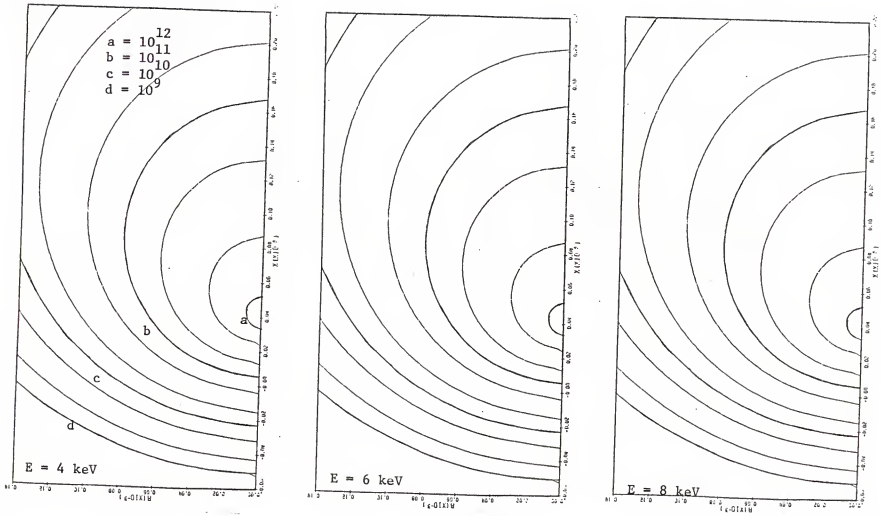


Figure 2.18. Contours of fit to normalized spatial yield spectrum for E = 4 keV, E = 6 keV, and E = 8 keV. E_o = 10 keV.

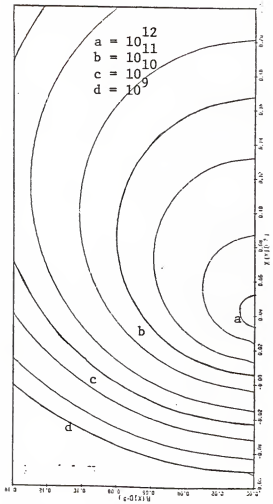


Figure 2.18. Contours of fit to normalized spatial yield spectrum for $E \leq 8$ keV. $E_o = 10$ keV. Pattern is essentially converged.

(2.4). Spatial yields for the various species are then found by summing over the appropriate branching ratios. By virtue of the device of separation of spectral energy dependence from spatial dependence mentioned at the end of the last section, the integral for $J_i(\rho,z,E_o)$ simplifies to

$$J_i(\rho,z,E_o) = \alpha_{io}(E_o)A_o(E_o)G_o(\rho,z,E_o) + \alpha_{i2}(E_o)A_2(E_o)G_2(\rho,z,E_o) + \\ + \alpha_{is}(E_o)A_s(E_o)G_s(\rho,z,E_o) \tag{2.30}$$

where

$$\alpha_{ij}(E_o) = \int_{E_i}^{E_o-E_i} p_i(E')C_jX^j(E',E_o)dE', \quad j = 0,2 \tag{2.31}$$

and $\alpha_{is}(E_o) = p_i(E_o)$.

Matters are made even simpler by our identification of the spatial dependence of the source term with the spatial dependence of the high spectral energy plume, i.e. by setting $G_o(\rho,z,E_o) = G_s(\rho,z,E_o)$, thereby reducing the number of separate spatial dependence terms in Eq. (2.30) to two.

Component g-values

The coefficients, $\alpha_{ij}(E_o)$, define associated g-values via the relation, $\alpha_{ij} = g_{ij}E_o/100$. For the sake of notation we may define $\alpha_{io,s} = \alpha_{io} + \alpha_{is}$ since only the sum of these two quantities is of interest. We may also define the quantity $\alpha_i = \alpha_{i2} + \alpha_{io,s}$. It is

the associated g-value, g_i which is generally referred to as "the" g-value, and which shall be referred to here as the total g-value. The idea of defining component g-values follows naturally from the Green-Singhal concept of separate spectral plumes.

In his Ph. D. thesis (1983) Rio calculated the total g-values of the various states as functions of E_o and displayed them graphically. From these results via the branching ratios, the g-values for the various species follow without too much trouble.

The total g-values (g_i) and high spectral component g-values ($g_{io,s}$) are graphed here in Fig. 2.19 for the eight individual species: e^-, H_2O^+, H^+, OH^+, H, OH, H_2, and O, and for the sum of ions. Note that the high spectral component dies off as E_o increases above 500 eV. This reflects the increasingly earlier spatial convergence, spectrally speaking, of the spatial yield spectrum with increasing E_o, noted and discussed in the previous section. Specifically, the spectral gate, $f(E,E_o)$, as a factor in the integrand of the probability integral, acts like a tunable high pass filter. As a result of this tuning over E_o, the ratio, $g_{io,s}/g_i$, $\uparrow 1$ as E_o decreases, and decreases to a small steady level, about 0.1, at higher E_o, as can be seen from Fig. 2.18.

At this point it is important that we recall our empirical result from chi square fitting of the data and graphical display that the short range of the high spectral plume relaxes as E_o increases. If this is a true result, it means that the effect of the high spectral plume on the relative profiles of the spatial yields is further decreased at higher E_o.

Charge Balance

Another matter comes to light in these graphs. This is the matter of charge balance. The electron yield, other than for contribution from ionizing decay of excited states, is calculated independently of the corresponding ion yields, namely directly from counting in the Monte Carlo calculation, and therewith the normalization, $N(E_o)$, in the deposition spectrum.

In these graphs, for every species except the electron, an uncorrected and a corrected value is shown. The uncorrected value is calculated according to prescription. The corrected value (i. e., corrected in the sense of maintaining the constraint of charge balance) is calculated according to a simple renormalization procedure described below.

Upon comparison of the g-value of ion pairs, obtained by summing the g-values of all three ion species, with the g-value of ion pairs implied from the g-value for the electron (subtracting out the primaries), a discrepancy is noted which is small at low energies but which increases from 200 eV and becomes significant. This is seen in Fig. 2.20 in which the corrected g-value for ion pairs is made to agree with the g-value for ion pairs implied by the g-value for electrons.

The source of the problem is not clear. It could be a result of misalignment of the total inelastic cross section with the sum of the individuals--or there may be a problem with the Monte Carlo program--one of inaccuracy in assignment of the two dimensional yield spectrum. This latter possibility can be discounted since this part of the code was

Figure 2.19. Total g-value and high spectral plume component for (a) the thermalized electron, (b) positive ions, (c) H_2O^+, (d) H^+, (e) OH^+, (f) H, (g) OH, (h) H_2 and (i) O.

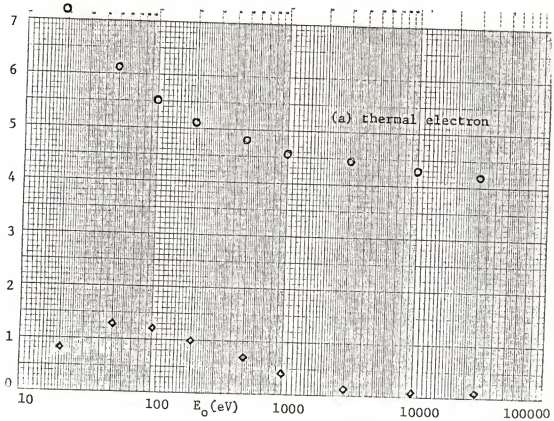


Figure 2.19 (a) thermal electron

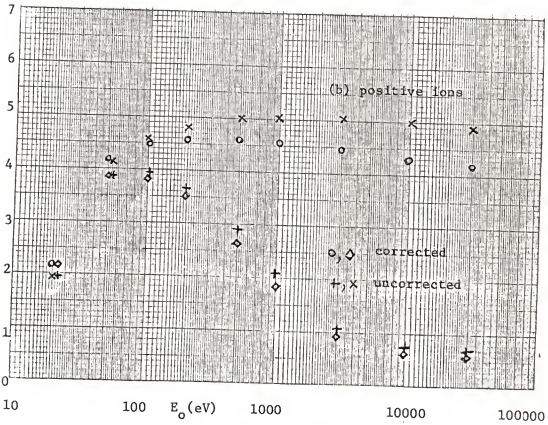


Figure 2.19 (b) positive ions

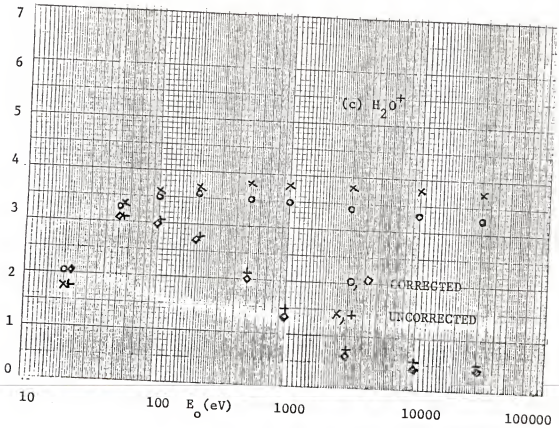


Figure 2.19 (c) H_2O^+

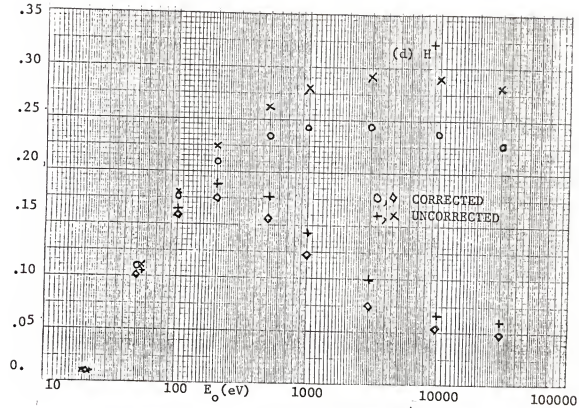


Figure 2.19 (d) H^+

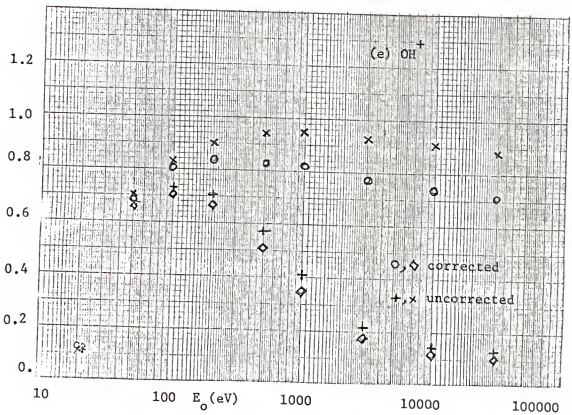


Figure 2.19 (e) OH^+

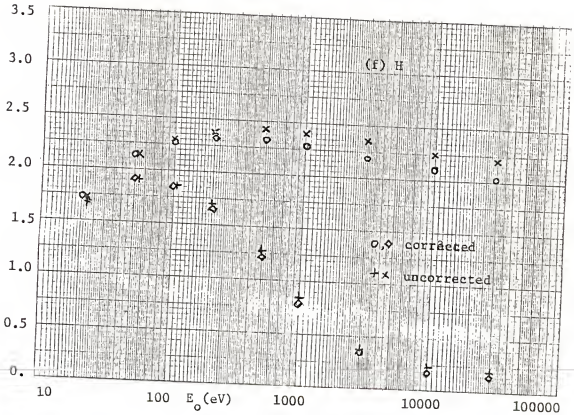


Figure 2.19 (f) H

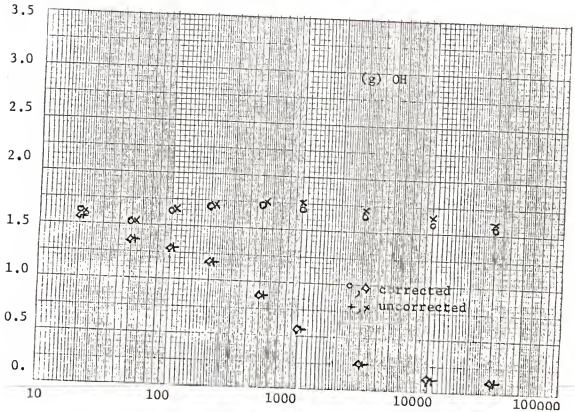


Figure 2.19 (g) OH

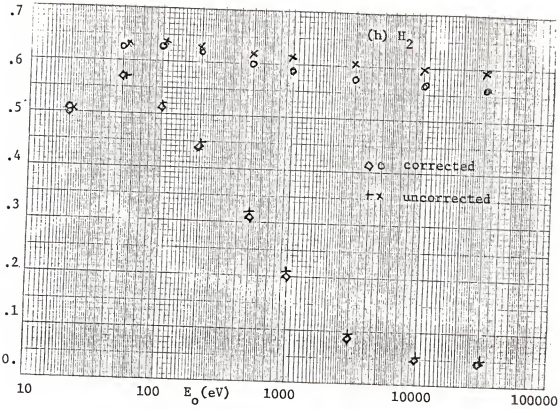


Figure 2.19 (h) H_2

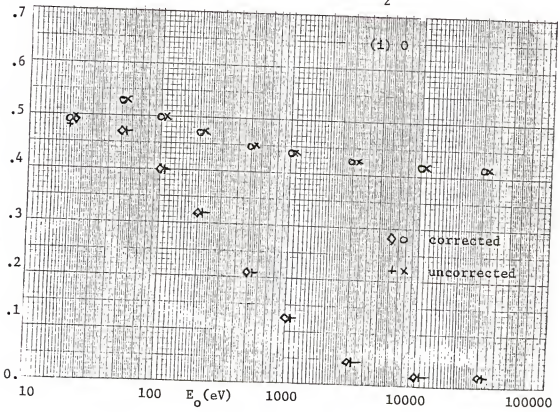


Figure 2.19 (i) O

checked out by Green, Garvey and Jackman (1977) against the modified discrete energy bin (MDEB) method of Peterson (1969) and was found to be in good agreement.

However, this problem need not deter us. Granted that if something is amiss with the ions, there may be reason to suspect the rest, however, the discrepancy is not great: 10% at 1 keV, 16% at 10 keV. Therefore, a little shifting around of values does not do any harm even at worst, and is probably better than that. The important thing sought is exact charge balance--as a constraint. The following corrective procedure therefore seems reasonable: renormalize the ionization states by the ratio $N(E_o) - 1$ divided by the total ion yield per incident electron as is.

Since the discrepancy in ev/ion pair is not very great, the corrective procedure outlined above would seem to be adequate to our purposes here. As can be seen from Fig. 2.19, the effect of the procedure on the three major species (other than the electron, which remains unaffected), namely H, OH, and H_2O^+, is about the same as for ev/ion pair in the case of H_2O^+ (the major ionic species), somewhat less for H, and nil for OH.

In Fig. 2.20 are graphed the (corrected) g-values of the post-recombinations yields assuming the approximation of globally instantaneous recombination of ion pairs (see Chapter IV), i.e., ignoring charge separation.

Figure 2.20. Total post-recombination g-value and high spectral plume component for (a) H and OH, and (b) H_2 and O assuming global instantaneity (see Chapter IV).

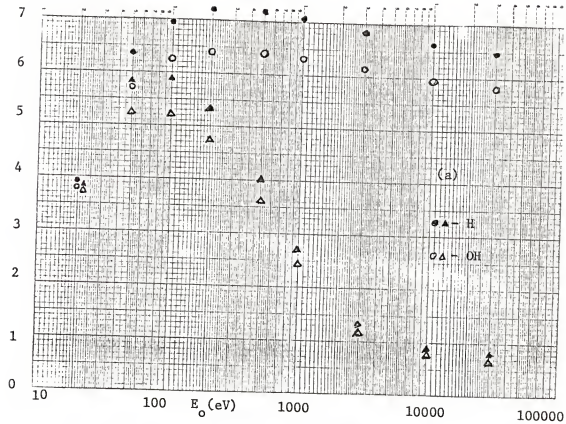


Figure 2.20 (a)

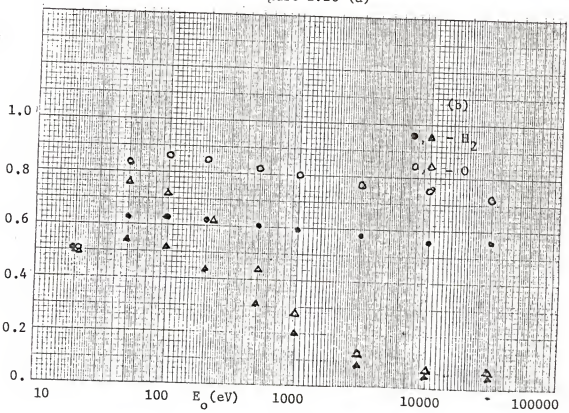


Figure 2.20 (b)

Charge Separation

The next matter that comes to our attention is charge separation. Noting the difference between the large high spectral plume component of the g-value for positive ions and the small value for the electron (this small value is a post-Monte Carlo result, and arises from the decay of certain excited states of H_2O (see Rio, 1983)), it is clear that charge separation is significant, and more so at lower incident energy. A good illustration of this is provided by Kupperman (1974) where representative profiles of $H_3O^+_{aq}$, OH, and e^-_{aq} are plotted for "typical" (? eV) incident energy for liquid H_2O.

The reason for mentioning charge separation, other than to call attention to one imporant feature of the g-values and component g-values, is to emphasize the sensitivity of the accuracy of their calculation to the accuracy of representation of the yield spectra. Specifically what is meant here is that the value of the high spectral plume g-value (taking the Green-Singhal approach) is highly sensitive to the spectral variation of $f(E,E_o)$. It would be advantageous, as a future direction for work in this effort, to extend the Monte Carlo data reduction to include numerical calculation of spatial yields along with spatial yield spectra so that definitive comparison of direct calculation with calculation via the intermediary of the fitted spatial yield spectra would be possible.

W-value

It is of interest to represent one particular g-value analytically, namely the low spectral plume component for electrons, $g_{e^-_d}$,

representing the contribution of the deposition spectrum. (Here the notation d rather than 2 is used to refer to the low spectral plume, since it is for the electron, and therefore arises from the deposition spectrum. This is done for the sake of formal consistency.) The quantity more frequently referred to in this context is the W-value, or ev/ion pair. From its definition, it follows that

$$g_{e^-d} = (100/E_o)\alpha_{e^-d} = (100/E_o)N(E_o).$$

We may define $g_{ip} = (100/E_o)(N(E_o) - 1)$, the g-value of ion-pairs which discounts the primaries. It follows that $W = 100/g_{ip}$ and, therefore, $W = E_o/(N(E_o) - 1)$.

Noting that $N(E_o)$ must fall to 1 as E_o decreases to $I = 12.6$ eV, the ionization threshold, and observing the near proportional LET limit, we can conveniently represent $N(E_o)$ by

$$N(E_o) = \begin{cases} 1 + 0.0415\,(E_o^{.965} - I^{.965}), & E_o > I \\ 1, & E_o < I \end{cases} \tag{2.32}$$

CHAPTER III
ANALYTIC PRELIMINARIES

Introduction

The purpose of this chapter is to gain some insight into the kinetics of both the ion and the neutral reactions and diffusion kinetics of the neutral reactions by abstracting to simpler, representative cases. It is possible to treat many of these cases analytically--either exactly or approximately. Numerical results are also made use of, and are obtained via a program written for this thesis, called DIFKIN (adapted from the BOAT code of Dash and Pergament (1978), see Appendices A and B), which calculates time dependent diffusion kinetics in spherical geometry.

In the case of pure kinetics both the case of an initial pulse and of a continuous pulse turned on at t=0 are discussed. This is for the most part for the sake of background, since these basic results are well known (for example, see Leu et al., 1973). The treatment of two body distinct species decay for continuous yield is, however, original, to the best knowledge of the author.

In order to clarify the role of diffusion in diffusion kinetics, the case of pure diffusion is first presented for the sake of background (in spherical geometry). The case of time dependent diffusion in axisymmetric geometry is discussed in Appendix C, although this work is as yet incomplete. Results for steady state diffusion, however, are presented and discussed.

For diffusion kinetics only the continuous pulse is discussed. We first consider two body decay of one species. The basic time dependent trends are identified and discussed. The asymptotic limits of the steady state solution are also identified and discussed. An analytic spline between these limits is identified and presented in Appendix D.

The case of two distinct species is considered next in a physically specific context, namely the recombination reaction, $H + OH + M \rightarrow H_2O + M$, in order that we might be able to isolate its effect in the corresponding calculated results for the full system later in Chapter VI.

The general case of diffusion kinetics of ν-body decay is also considered as an aside of theoretical interest in Appendix E. The concept of an inverse length associated with the reaction rate and diffusion coefficient is generalized, and the trend with ν is investigated.

Kinetics

Single species decay. We begin with a simple result -- the decay of a single species by reaction with itself. We may first consider the general ν-body case and then specialize. Denoting the concentration by c, the "yield rate" or source term by y, and reaction rate by k, the equation in the pure kinetic case is

$$dc/dt = -\nu k c^{\nu} + y \tag{3.1}$$

which for continuous source $(y \neq 0)$ becomes

$$d\gamma/d\tau = 1 - \gamma^{\nu} \tag{3.2}$$

upon making the transformations $\gamma = \sqrt[\nu]{\nu k/y}\, c$ and $\tau = yt/\sqrt[\nu]{y/\nu k}$. This is easily solved in the cases $\nu = 1$ and $\nu = 2$ to give respectively

$$c = \frac{y}{k}\,(1 - e^{-kt}) \tag{3.3}$$

and

$$c = \sqrt{\frac{y}{2k}}\,\tanh\sqrt{2ky}\;t. \tag{3.4}$$

In the general case the inverse solution is easily found by expansion in geometric series and integrating:

$$\tau = \sum_{j=0}^{\infty} \frac{1}{\nu j + 1}\,\gamma^{\nu j+1}. \tag{3.5}$$

The trend of the solution in ν is shown by the graph in Fig. 3.1 in which $\gamma(\tau)$ is plotted versus τ for a sequence of values of ν. The trend is as one would expect intuitively, namely, that as the number of molecules (or, in general, fractions of units) which must come together to form a reaction increases, the approach to saturation becomes more abrupt in time. This is seen already in the cases $\nu = 1$ and $\nu = 2$. The value of γ at reduced time $\tau = 1$ (at which the asymptotes intersect) is $1-1/e$ in the case $\nu = 1$ and $1 - 2/(e^2(1 + 1/e^2))$ in the case $\nu = 2$. In general for $\nu \gtrsim 1$ a 'reaction time' or 'transition time' may be defined at $\tau \approx 1$. The transition is fairly abrupt

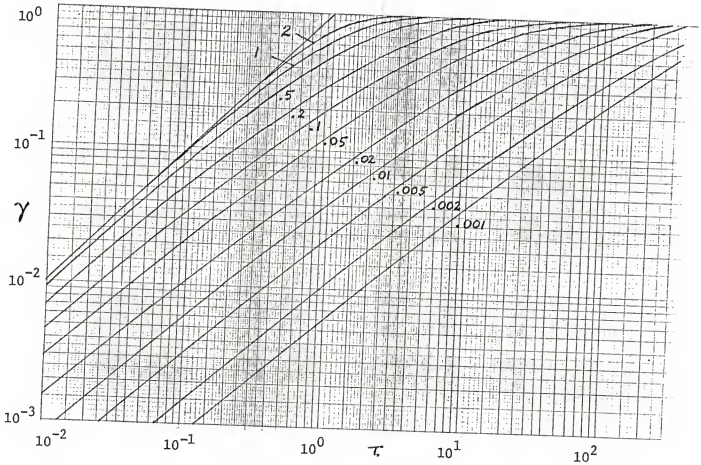


Figure 3.1. $\gamma(\tau)$ vs. τ for ν = .001, .002, .005, .01, .02, .05, .1, .2, .5, 1, 2.

between beginning and end. For $0 < \nu \lesssim 1$ onset is gradual while end of transition is abrupt (in logarithm of time).

The initial pulse case can be solved explicitly, and is given by

$$c = \begin{cases} \dfrac{c_o}{\left(1 + \nu(\nu-1)c_o^{\nu-1}kt\right)^{1/(\nu-1)}}, & \nu \neq 1,\ \nu > 0 \\ c_o e^{-kt}, & \nu = 1 \end{cases} \tag{3.6}$$

These solutions are plotted in Fig. 3.2 as c/c_o vs. $c_o^{\nu-1}kt$ for a sequence of values of ν.

The curve for $\nu = 1$ is a tangential envelope of those for $\nu > 1$. The trend with ν for $\nu > 1$ is analogous to that in the case $y \neq 0$, only instead of more abrupt here the trend is towards more gradual. This is because here the system is simply decaying, while the decay is offset by the competing effect of the continuous source term. Thus, at first, decay is insignificant, only the effect of the source term is seen. Finally because of the built up concentration, decay has gained strength, and the balance shifts. This time can be called a 'critical' time.

In the pure decay (initial pulse) case, an interesting result obtains for $\nu < 1$. That is, that the decay accelerates until an endpoint time is reached at which the material is completely consumed. The effect of stoichiometric factor is irrelevant to this, only the power law matters.

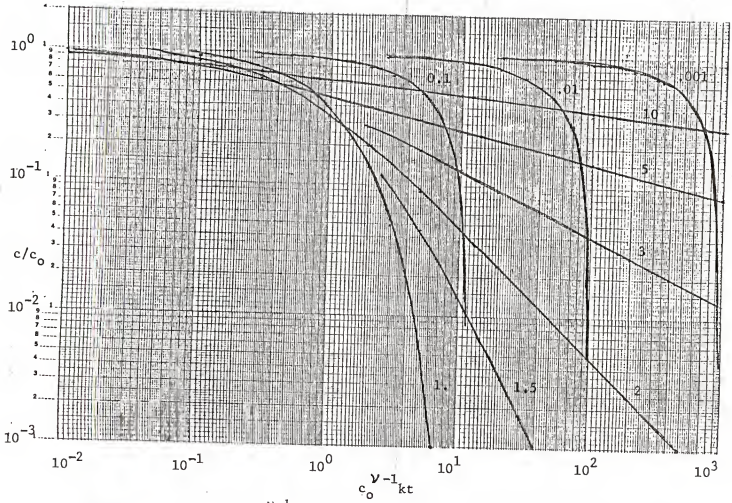


Figure 3.2. c/c_o vs. $c_o^{\nu-1}kt$ for ν = .001, .01, .1, 1, 1.5, 2, 3, 5, 10.

Two body two species decay. We next consider the case of coupled two body decay between two distinct reactants. The kinetic equations are given by

$$dc_1/dt = -kc_1c_2 + y_1$$

$$dc_2/dt = -kc_1c_2 + y_2 \tag{3.7}$$

Let us first consider the initial pulse case. Setting $y_1 = y_2 = 0$, we at once obtain $c_1 = c_{10} + (c_2 - c_{20})$. The equations thereby decouple to give

$$dc_1/dt = k(c_{10} - c_{20})c_1 - kc_1^2$$

$$dc_2/dt = -k(c_{10} - c_{20})c_2 - kc_2^2 \tag{3.8}$$

The solution is found by integration and is given by

$$c_1 = \frac{c_{10}(c_{10} - c_{20})}{c_{10} - c_{20}e^{-k(c_{10} - c_{20})t}}$$

$$c_2 = \frac{c_{20}(c_{10} - c_{20})}{c_{10}e^{k(c_{10} - c_{20})t} - c_{20}} . \tag{3.9}$$

This result is in agreement with intuition--the majority species falls off to the initial difference while the minority species is completely destroyed. The asymptotic limit (Eq. (3.6), $\nu = 2$) is approached

as $c_{10} - c_{20} \to 0$ or, more generally, as $(c_{10} - c_{20})/(c_{10} + c_{20}) \to 0$ if we replace c by c/2 to reflect counting. In the opposite limit, $(c_{10} - c_{20})/(c_{10} + c_{20}) \to 1$, the asymptotic limit (Eq. (3.6), $\nu = 1$) is approached for c_2, with k in this equation replaced by kc_{10}, where this k is from Eq. (3.9). Thus, c_1 is effectively a constant background, while c_2 undergoes effective one body decay. This equation was first investigated by Verhulst (1838) in the study of saturation of populations (see Green and Burki, 1974).

We next consider the continuous pulse case. Making the transformation $a_1 = (c_1 + c_2)/2$ and $a_2 = (c_1 - c_2)/2$, the equations transform to

$$\begin{aligned} da_1/dt &= -k(a_1^2 - a_2^2) + (y_1 + y_2)/2 \\ da_2/dt &= (y_1 - y_2)/2. \end{aligned} \tag{3.10}$$

The second of these equations immediately integrates to give

$$a_2 = (y_1 - y_2)t/2 \tag{3.11}$$

which upon substitution into the other equation yields

$$da_1/dt = -k(a_1^2 - (y_1 - y_2)^2 t^2/4) + (y_1 + y_2)/2. \tag{3.12}$$

We make the transformation, $x = kt$, yielding

$$da_1/dx = -a_1^2 + \left(\frac{y_1 - y_2}{2k}\right)^2 x^2 + \frac{y_1 + y_2}{2k}. \tag{3.13}$$

This is a first order differential equation of Ricatti type for which the transformation, $a_1 = u'/u$, transforms the equation to a second order linear differential equation. We obtain

$$u'' = (B^2x^2 + C)u \tag{3.14}$$

where $B = (y_1 - y_2)/2k$ and $C = (y_1 + y_2)/2k$. Other than for the sign of C, this is just the Schroedinger equation for a simple harmonic oscillator. Following the development in Eisberg (1961), we may transform one more time, setting $\alpha^2 = C/B = (y_1 + y_2)/(y_1 - y_2)$ and $\xi = \sqrt{B}\ x = \sqrt{(y_1-y_2)k/2}\ t$ to obtain

$$u'' = (\xi^2 + \alpha^2)u. \tag{3.15}$$

The solution is found by making the substitution $u = He^{\xi^2/2}$, yielding the differential equation for H,

$$H'' + 2\xi H' + (1 - \alpha^2)H = 0 \tag{3.16}$$

for which the solution is most conveniently found by means of a power series. The recursion relation is given by

$$h_{n+2} = \frac{\alpha^2 - 1 - 2n}{(n+1)(n+2)}\, h_n,\ n \geq 0. \tag{3.17}$$

The initial condition $a_1 = 0$ implies that $h_1 = 0$; h_o is only required not to be zero, and is arbitrary as it scales out.

Solving now for a_1, we obtain

$$a_1 = (du/dx)/u = \sqrt{B}\,(du/d\xi)/u$$

$$= \sqrt{B}(\xi + H'/H) \tag{3.18}$$

$$= \frac{(y_1 - y_2)t}{2} + \sqrt{\frac{y_1 - y_2}{2k}}\;\frac{H'(\xi;\alpha)}{H(\xi;\alpha)}$$

where $\xi = \sqrt{(y_1 - y_2)k/2}\;t$ and $\alpha^2 = (y_1 + y_2)/(y_1 - y_2)$ as noted above. Noting that $h_2/h_o = (\alpha^2 - 1)/2$, it follows that $a_1 \sim (y_1 + y_2)t/2$ for $t \sim 0$. From the fact that $H'/H \to 0$ as $\xi \to \infty$ (to easily see this, consider the case where H truncates to a polynomial) it follows that $a_1 \to (y_1 - y_2)t/2$ as $t \to \infty$. Therefore $c_1 \sim y_1 t$ and $c_2 \sim y_2 t$ for $t \sim 0$ and $c_1 \sim (y_1 - y_2)t$ and $c_2 \to 0$ as $t \to \infty$, as we might intuitively expect.

From this we see that the quantity,

$$g(\xi;\alpha) = H'(\xi;\alpha)/[(\alpha^2 - 1)\xi H(\xi;\alpha)]$$

gates the solution between its asymptotic limits in t. The essential information of the solution is therefore seen to be contained in this function in its most meaningful form. In order to get a better look at $g(\xi;\alpha)$ we may define an alternative dimensionless time, $\eta = \sqrt{ky_2}\;t$, and a new parameter, $\Delta = (y_1 - y_2)/y_2$. Note, η and Δ are given in terms of ξ and α by $\Delta = (\alpha^2 - 1)/2$ and $\eta = \sqrt{2/\Delta}\;\xi$. The purpose of this new variable, η, is to provide a fixed point of reference while varying y_1 while keeping y_2 fixed (thinking of y_1 as the majority species).

Equation (3.16) then transforms to

$$\tilde{H}'' + \Delta\eta\tilde{H}' - \tilde{H} = 0 \tag{3.20}$$

where we have defined $\tilde{H}(\eta;\Delta) = H(\xi;\alpha)$ and $\tilde{g}(\eta;\Delta) = g(\xi;\alpha)$. Note that

$$\tilde{g}(\eta;\Delta) = \frac{1}{\eta}\frac{\tilde{H}'(\eta;\Delta)}{\tilde{H}(\eta;\Delta)} .$$

We are now in a somewhat better position to investigate the asymptotic limits in Δ of the behavior of $\tilde{g}$. Referring to Eq. (3.20) it follows at once that $\tilde{H}(\eta;\Delta) = \cosh\eta$ (from which we obtain $\tilde{g}(\eta;\Delta) = \tanh\eta/\eta$) in the limit $\Delta \to 0$, in agreement with Eq. (3.4). In the limit $\Delta \to \infty$ the gate limit at $\eta \sim 0$ is retained by the factor in the middle term in Eq. (3.20). We consider the asymptotic behavior at the other end, namely as $\Delta \to \infty$. Making the Ansatz, $H \propto \eta^{\rho}$, $\rho < 2$, it follows that Eq. (3.20) takes on the asymptotic form

$$\Delta\eta\tilde{H}' - \tilde{H} = 0 \tag{3.21}$$

as $\eta \to \infty$, from which we obtain $\rho = 1/\Delta$, implying $\tilde{g}(\eta;\Delta) \approx 1/\Delta\eta^2$.

Evaluating $\tilde{g}(\eta;\Delta)$ by means of the power series expansion for a representative sequence of values of Δ, the results are graphed in Fig. 3.3. The asymptotic limit as $\Delta \to 0$ is seen to carry down to at least two orders of magnitude in g for $\Delta < .01$. The asymptotic limit as $\Delta \to \infty$ is seen to hold in all applicable cases ($\Delta > 0.5$). In the

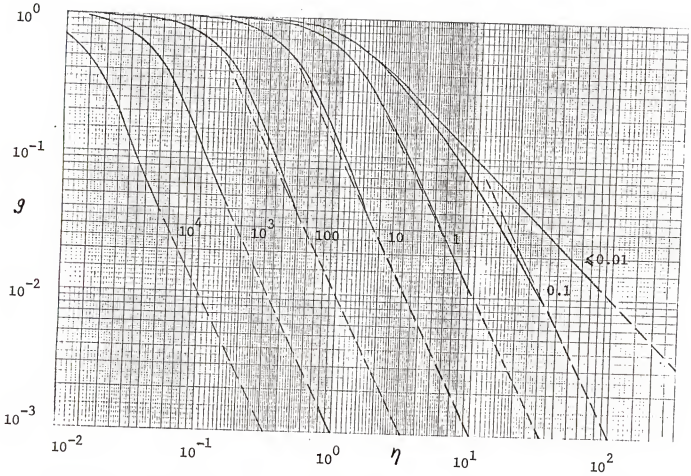


Figure 3.3. $\tilde{g}(\eta;\Delta)$ vs. η for Δ = 0 - 0.01, 0.1, 1.0, 10, 100, 1000 and 10^4.

intermediate region ($0 < \Delta < 0.5$) the limits of precision of the calculation suggest that this limit may also hold here as well but do not go far enough to confirm it.

We may define a dimensionless reaction time, η_c, most conveniently as the point of intersection of the asymptotes in g. For $\Delta < 1$, $\eta_c \sim 1$. For $\Delta \gtrsim 1$, $\eta_c \approx 1/\sqrt{\Delta}$. Due to the effect of smooth transition, the prescription in terms of intersection of aymptotes is defaulted in the transition interval in η. The retreat of η_c to zero as Δ increases is in agreement with physical intuition--namely, that for a fixed concentration of scavengee, as the scavenger concentration increases, the quickness with which the scavengee is removed increases.

Finally, we may state these results in conventional units:

$$\tau_c \approx 1/\sqrt{ky_2}\ ,\ 0 < \Delta \lesssim 1 \quad (y_2 < y_1 \lesssim 2y_2)$$

$$\tau_c \approx 1/\sqrt{k(y_1 - y_2)},\quad \Delta \gtrsim 1\ (y_1 \gtrsim 2y_2)\ . \tag{3.22}$$

Diffusion

In this section basic diffusion results are reviewed in order to identify the role displayed by diffusion in diffusion kinetics, and also to provide an independent check on the accuracy of the diffusion component of the computer program, DIFKIN. More about the program itself is to be found in Appendix A.

Only the case of spherical geometry is considered. For higher incident energies where more elongated contours obtain, the spherical approximation becomes less adequate and a full two dimensional

calculation is desirable. Efforts to carry out such a program, which are unfinished, are described in Appendix B. At lower incident energies, the contours are less elongated, and the spherical approximation is adequate.

For the sake of application, an analytic approximation is devised for the time dependent solution to the diffusion equation in spherical geometry. Finally, the characteristic time for convergence of the solution to steady state is discussed in the context of providing an approximate analytic representation of the inverse solution near in the approach to steady state.

The diffusion equation is given by

$$\frac{\partial c}{\partial t}(\vec{r},t) = D\nabla^2 c(\vec{r},t) + 4\pi D\rho(\vec{r},t) \tag{3.23}$$

where $4\pi D\rho(\vec{r},t)$ is the source term. We will condense this into the single dependent variable $y(\vec{r},t)$. Adequate derivations of the diffusion equation in terms of differential elements of mass flux are given in various texts, such as Reif (1965).

Morse and Feshbach (1953) give the solution to the zero initial value problem by

$$c(\vec{r},t) = \iint g_D(R,\tau)\rho(\vec{r}_o,t)\, d\vec{r}_o dt_o \tag{3.24}$$

where $g_D(R,\tau)$ is the associated Green's function, given by

$$g_D(R,\tau) = \frac{4\pi D}{(2\sqrt{\pi D\tau})^3} \quad e^{-R^2/4D\tau}\theta(\tau) \tag{3.25}$$

where $R = ||\vec{r} - \vec{r}_o||$, $\tau = t - t_o$.

For the spherical case we may set $R = \sqrt{r^2 - 2rr_o\mu_o + r_o^2}$ where $\mu_o = \cos\theta_o$ and $d\vec{r}_o = r_o^2 dr_o d\mu_o d\phi_o$. Integrating over μ_o and ϕ_o, Eq. (3.24) simplifies to

$$c(r,t) = \int_0^t \frac{dt_o}{\sqrt{\pi D\tau}} \int_0^\infty dr_o \; y(r_o,t_o) \frac{r_o}{r} \left[e^{-\frac{(r-r_o)^2}{4D\tau}} - e^{-\frac{(r+r_o)^2}{4D\tau}}\right] \tag{3.26}$$

We set $y(r,t) = Ae^{-\beta r}f(t) = (\beta^3 N/8\pi)e^{-\beta r}f(t)$, in line with the spatial dependence of radiological yields as determined in Chapter 2. For this spatial dependence of $y(r,t)$, the integral over r_o is analytic, and $c(r,t)$ can be found by the single time integral,

$$c(r,t) = \frac{A}{2r}\int_0^t dt_o \quad f(t_o)\Big[(2\beta D\tau + r)e^{\beta(\beta D\tau + r)}\mathrm{erfc}\Big(\frac{2\beta D\tau + r}{\sqrt{4D\tau}}\Big)$$

$$- (2\beta D\tau - r)e^{\beta(\beta D\tau - r)}\mathrm{erfc}\Big(\frac{2\beta D\tau - r}{\sqrt{4D\tau}}\Big)\Big] \tag{3.27}$$

The first term in the integrand is unusable for numerical calculation in its present form for $\beta(\beta D\tau + r) > 174$, due to overflow in the argument of the exponent, the second term for $\beta(\beta D\tau - r) > 174$. In either case, the asymptotic expansion (Dwight, 1961) must be used to overcome this problem - the implied product of a very large and a very small number then becomes explicit and cancels out. These two terms are then given by

$$(2D\beta\tau + r)\, e^{\beta(\beta D\tau + r)}\ \mathrm{erfc}\ \frac{2\beta D\tau + r}{\sqrt{4D\tau}} =$$

$$\sqrt{4D\tau/\pi}\ \ e^{-r^2/4D\tau}\ S\left(\frac{2\beta D\tau + r}{\sqrt{4D\tau}}\right) \tag{3.28a}$$

and

$$(2D\beta\tau - r)\, e^{\beta(\beta D\tau - r)}\ \mathrm{erfc}\ \frac{2\beta D\tau - r}{\sqrt{4D\tau}} =$$

$$\mathrm{sgn}(2\beta D\tau - r)\ \sqrt{4D\tau/\pi}\ \ e^{-r^2/4D\tau}\ S\left(\frac{2\beta D\tau - r}{\sqrt{4D\tau}}\right)$$

$$+ (1 - \mathrm{sgn}(2\beta D\tau - r))(2\beta D\tau - r)\, e^{\beta(\beta D\tau - r)} \tag{3.28b}$$

where

$$S(x) = \sum_{n=0}^{\infty} \frac{(-)^n (2n)!}{(2x)^{2n}}$$

Implementing these replacement forms where needed, the integral can be calculated as a single integral numerically everywhere (in (r,t)).

For the initial pulse, $f(t) = \delta(t)$, and the solution is analytic. For the continuous pulse turned on at $t = 0$, $f(t) = \theta(t)$ and the solution reduces to a single integral in time. In these calculations the variable mesh multiple integration program of Coldwell (private communication, 1979) has been used. This program is relatively cheap, quite accurate, provides error estimates, and is convenient to use.

Calculating c(r,t) for the continuous pulse via DIFKIN, agreement is obtained at all points r and t to within a percent. The solution c(r,t) for the continous pulse is graphed in Fig. 3.4 as a time sequence

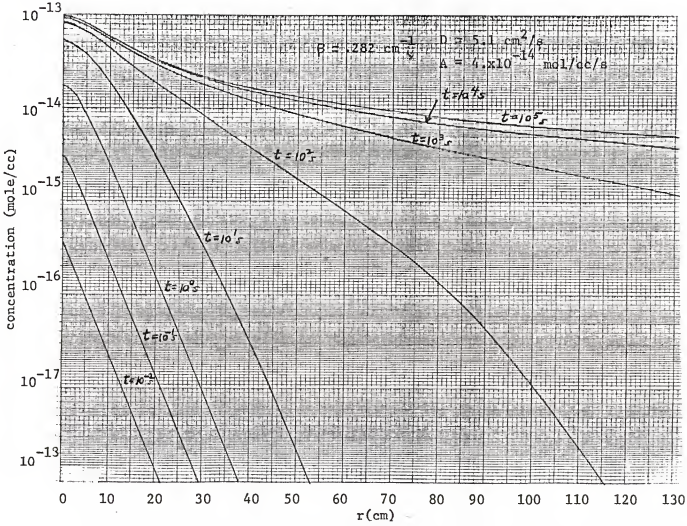


Figure 3.4. Time sequence of radial profiles for pure diffusion in spherical geometry.

of radial profiles. This sequence graphically displays the convergence upon the steady state profile, $c_{st}(r)$, which is found by repeated quadrature:

$$c_{st}(r) = \frac{A}{D\beta^2}\left[\frac{2(1-e^{-\beta r})}{\beta r} - e^{-\beta r}\right] \tag{3.29}$$

It is useful to define a reduced distance, $r' = \beta r$ and a reduced time, $t' = D\beta^2 t$. We may also introduce a reduced concentration, c', by the definition, $c' = c/(A/D\beta)^2$, so that steady state peak value is 1.

Regarding the steady state solution, we note that the distance at which its asymptotic form $c'_{st}(r') \approx 2/r'$ equals the peak value of the exact solution, is twice the e-folding interval. The inflection point occurs further out, at 3.38 times the e-folding interval, followed by the half width at 3.72. These distances delineate the diffuse boundary of what we may call the steady state core to reflect the fact that steady state is converged on fully two orders of magnitude earlier within it than in the surrounding limb. This is clearly indicated in Fig. 3.5.

The relative suddenness of arrival of steady state within the central core reflects the simple fact that this is the location of the source. The core is essentially coterminous with the range of the source--at $r' = 3.5$ the source value is down to 3% of peak.

It is possible to analytically approximate $c'(r',t')$ fairly closely for all r' and t' by observing the early asymptotic limit,

$$c'(r',t') \sim t'e^{-r'} \text{ for } (r'^2 + r_o'^2)/4t' \gg 1 \tag{3.30}$$

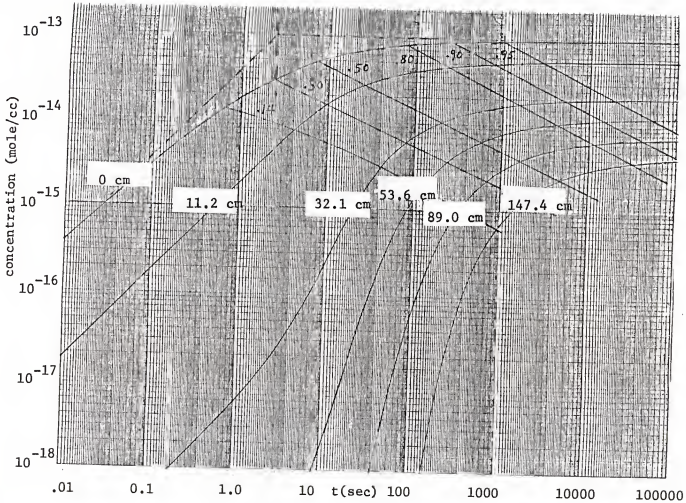


Figure 3.5. Time course at selected radial distances for pure diffusion in spherical geometry. Isocontours of constant p are overlaid.

where r' is of the order of unity and, of course Eq. (4.29). Splining these limits together by means of a modification of the Green's function, we arrive at

$$c'(r',t') = c'_{st}(r')c'_o(t')F + (1 - F)\left[(1-G)t'' + gc'_o(t')\right]e^{-r'}$$

where $F = F(r',t'')$ and $G = G(r',t'')$

and $F(r',t'') = G(r',t'') = e^{-r'^2/4t''}$ (3.31)

where $t'' = t'/(1 + \alpha_1(4t'/(r'^2 + r_o'^2))^{\alpha_2}]$

where $\alpha_1 = 0.56$, $\alpha_2 = 0.65$ and $r'_o = 1.40$ and where $c'_o(t) = c'(0,t')$ is easily represented by

$$c'_o(t') = t'/(1 + 1.40\ t'^{1/2} + t'). \qquad (3.32)$$

The accuracy of this fit to $c'(r',t')$ is illustrated in Figs. 3.16a and b where it has been applied to the time dependent concentration of H and OH radical in the late chemistry case where the effect of chemistry on initial yield species is nil. Its usefulness is further illustrated in Fig. 3.16c (for discussion see associated text).

In order to get a better idea of convergence time, $c(r,t)$ is regraphed in Fig. 3.5 as a family of time courses at selected radial distances on which isocontours of convergence to fraction p of steady state value have been overlaid. Bearing the asymptotic form of the solution (Eq. 3.28) in mind, we approximately analytically characterize these isocontours by

$$t'(r',p) \approx a_1(p)r'^2/4 + a_2(p) \tag{3.33}$$

where $a_1(p) \approx (1 - p)^2$ and $a_2(p) \approx 1.2(1 - (1-p)^{1.5})/(1-p)^2$.

This approximate characterization of the inverse solution, $t'(r',p)$, in the convergence limit progressively loses accuracy for $p < .25$, and is not intended to be correct for $p > .95$, although it may be good somewhat beyond that. The asymptote intersection point for $r' = 0$ occurs at $t' = 1$. From either Eq. (3.32) or (3.33) it follows that $p' \approx 0.3$ at this point, i.e. at $t' = 1$. This may serve as a suitable definition of diffusion convergence time, which we will denote by τ_d.

Diffusion Kinetics

In this section we consider the diffusion kinetics of very simple systems of one and two body decay of one species (in an inert medium) and of two body decay of two species. Possible reaction contexts in which these kinetic modes are applicable are

$$S_1 \xrightarrow{k} S_2 + \cdots \tag{3.33.1}$$

or

$$S_1 + M \xrightarrow{k'} S_2 + M + \cdots \tag{3.33.1.M}$$

and

$$S_1 + S_2 \xrightarrow{k} S_3 + \cdots \tag{3.33.2}$$

or

$$S_1 + S_2 + M \xrightarrow{k'} S_3 + M + \ldots \qquad (3.33.2.M)$$

respectively. In the second and third body cases (catalysis by M) the effective one or two body reaction rate coefficient, respectively, is given by $k = C_M k'$.

The corresponding diffusion kinetic equations are given respectively by

$$\partial c_1/\partial t = D_1 \nabla^2 c_1 - kc_1 + y_1 \qquad (3.34.1.1)$$

$$\partial c_i/\partial t = D_i \nabla^2 c_i + kc_1 + y_i, \; i \geq 2 \qquad (3.34.1.2)$$

and

$$\partial c_1/\partial t = D_1 \nabla^2 c_1 - kc_1 c_2 + y_1 \qquad (3.34.2.1)$$

$$\partial c_2/\partial t = D_2 \nabla^2 c_2 - kc_1 c_2 + y_2 \qquad (3.34.2.2)$$

$$\partial c_i/\partial t = D_i \nabla^2 c_i + kc_1 c_2 + y_i, \; i \geq 3 \qquad (3.34.2.3)$$

where, in Equations (3.34.1.2) and (3.34.2.3) it has been assumed that the product species are inert and do not react further.

Only the case of continuous pulse source terms turned on at t=0 is considered. In both single body and two body cases we take $y_i(r) = A_i e^{-\beta r}$. We may start with the single body case first.

Single Body Decay

For comparison we recall the time dependence for the pure kinetic case given by Eq. (3.3). The appropriate point at which to make this comparison is r=0. We may table this result momentarily, and next note the spatial dependence of the steady state solution, for which Prof. Green has provided the derivation.

Setting $C_1 = C = G/r$, $B = A/D$ and $\kappa^2 = k/D$, Eq. (3.34.1.1) in the steady state transforms into

$$G'' - \kappa^2 G + rBe^{-\beta r} = 0 \tag{3.35}$$

for which the solution is given by

$$G = \frac{2B\beta}{(\beta^2-\kappa^2)^2}\left[e^{-\kappa r} - e^{-\beta r}\right] - \frac{Bre^{-\beta r}}{\beta^2-\kappa^2} \tag{3.36}$$

wherefore

$$C = \frac{2B\beta}{(\beta^2-\kappa^2)^2 r}\left[e^{-\kappa r} - e^{-\beta r}\right] - \frac{B\ e^{-\beta r}}{\beta^2-\kappa^2} \tag{3.37}$$

Note the reduction to the case of pure diffusion for $\kappa = 0$. The critical case $\beta = \kappa$ is found by taking the limit $\beta-\kappa \to 0$, and is given by

$$C = \frac{B\ e^{-\beta r}}{4\beta^2}(1 + \beta r) \tag{3.38}$$

We consider the following three cases: (1) $\beta = .25\ \text{cm}^{-1}$, $\kappa = .25\ \text{cm}^{-1}$, (2) $\beta = .25\ \text{cm}^{-1}$, $\kappa = .50\ \text{cm}^{-1}$, and (3) $\beta = .50\ \text{cm}^{-1}$,

$\kappa = .25\ cm^{-1}$. The value of D used is 1827 cm^2/sec, the binary diffusion coefficient of OH in H_2O at T = 400 K for medium density $6x10^{15}$ molec/cc. The values of k implied then by κ and D are 114.19 sec^{-1} and 456.75 sec^{-1}, equal to $D\beta^2$ and $4D\beta^2$, respectively, thus equal to $1/\tau_d$ and $4/\tau_d$, respectively, (see preceeding section). In Fig. 3.6 the time dependence at the point r=0 as found via DIFKIN is plotted for these three cases along with the pure kinetic case for comparison. The difference between the results for cases (2) and (3) which should and do approach the same steady state limit is interesting. Agreement to this point is to within a few percent.

In Fig. 3.7 the steady state profiles are plotted along with numerical profiles at t = 2 sec, 2 sec and 0.5 sec, the last time calculated for cases (1), (2) and (3), respectively. The agreement is almost exact. It is interesting to note the exponential fall off of these steady state profiles. This reflects the independence of the logarithmic rate of single body decay on concentration while the logarithmic rate of diffusion (the so-called "diffusion velocity"[1]) is independent of concentration (and can therefore balance the logarithmic decay rate) only for exponential fall off.

---

[1]Diffusion "velocity" is defined by

$$V_i = -D_i \frac{1}{C_i} \frac{\partial C_i}{\partial r}$$

where D_i is the binary diffusion coefficient of species i through the medium (Kanury, 1975). The significance is that D is defined as negative the ratio of particle flux, Γ, to concentration gradient. Therefore $\Gamma = CV$.

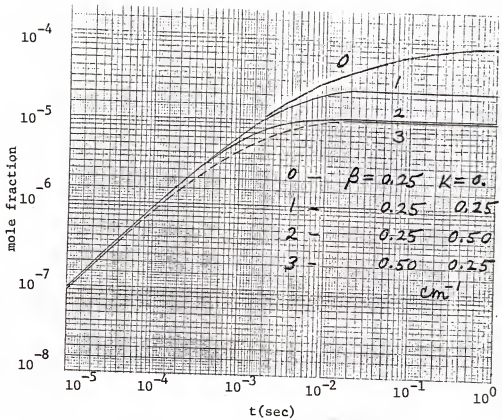


Figure 3.6. Time course for single body decay at r = 0. Three cases and pure diffusion shown for comparison.

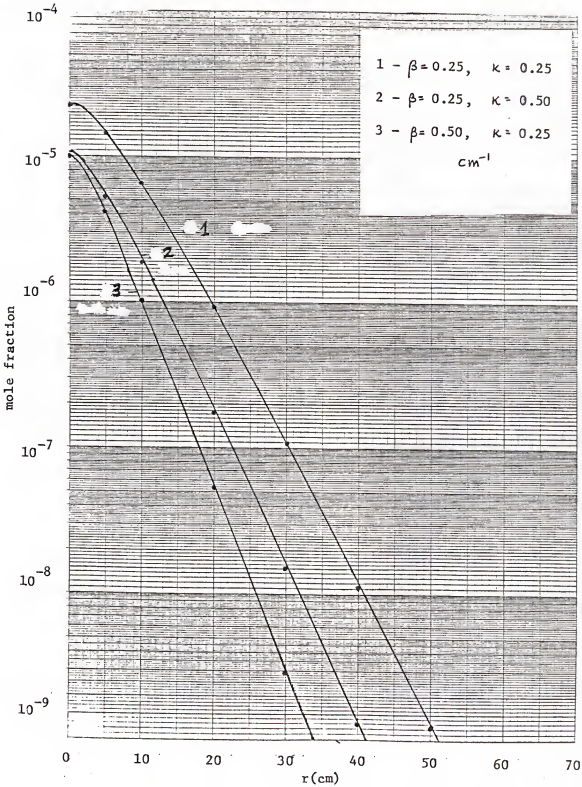


Figure 3.7. Steady state profiles for single body decay. Three cases as in Fig. 3.6.

In Figs. 3.8-10 time sequences of the radial profiles have been plotted for all three cases. Again, noting the independence of logarithmic rate of single body decay on concentration, we observe in the two cases where the chemistry is as fast as the diffusion at the center ($\kappa \geq \beta$) that the convergence is essentially simultaneous at all spatial points. In the case in which the chemistry is slower than the diffusion at the center, this is seen not to be the case. This is because the early time $e^{-\beta r}$ fall off is relaxing to the later time $e^{-\kappa r}/r$ fall off. The trend towards the pure diffusion limit is obvious. In the fast chemistry case, the early time $e^{-\beta r}$ fall off remains seated. With a little effort a suitable analytic spline could be found to patch early and later time dependences together, and thereby approximate the time dependent solution, $c(r,t)$.

Two Body Decay of One Species

We next turn our attention to the two body case. We first consider the case of two body decay of one species with itself. To reflect counting (stoichiometry) the destruction term is multiplied by two:

$$\frac{\partial C}{\partial t} = D\nabla^2 C - 2kC^2 + y \tag{3.39}$$

We again use D = 1827 cm /sec and β = .25 cm^{-1}, and we use the following four values of k: 1.08×10^{13} cc/mole/sec, 6.31×10^{13} cc/mole/sec, 1.08×10^{15} cc/mole/sec and 1.08×10^{17} cc/mole/sec. The value of A is 1.03×10^{-10} mole/cc/sec. The reaction times for pure kinetics at r=0 implied by these numbers, using Eq. (4.4) are .021 sec, .0088 sec,

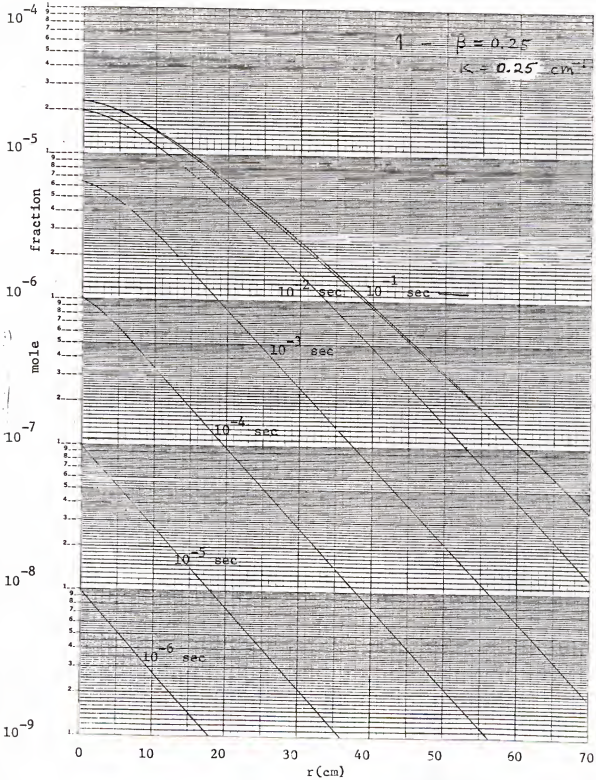


Figure 3.8. Time sequence of radial profiles for single body decay, $\beta = .25\ cm^{-1}$, $\kappa = .25\ cm^{-1}$.

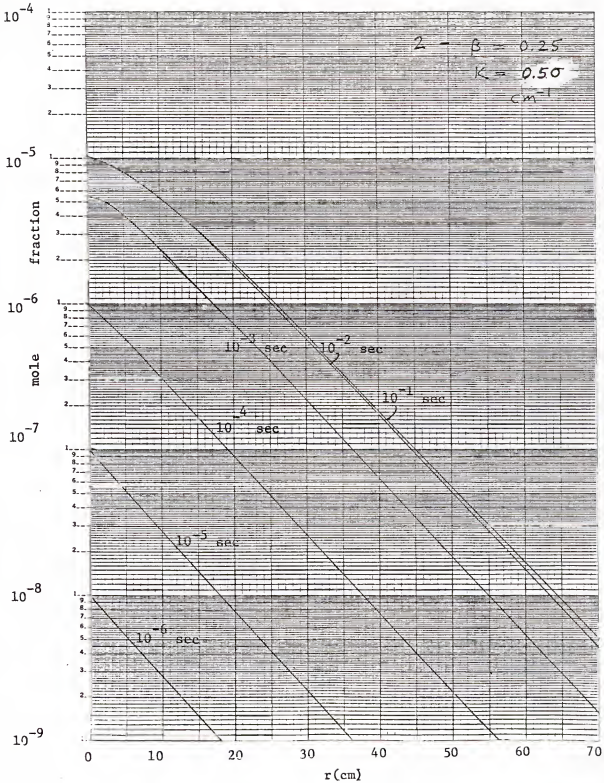


Figure 3.9. Time sequence of radial profiles for single body decay, $\beta = .25\ cm^{-1}$, $\kappa = .50\ cm^{-1}$.

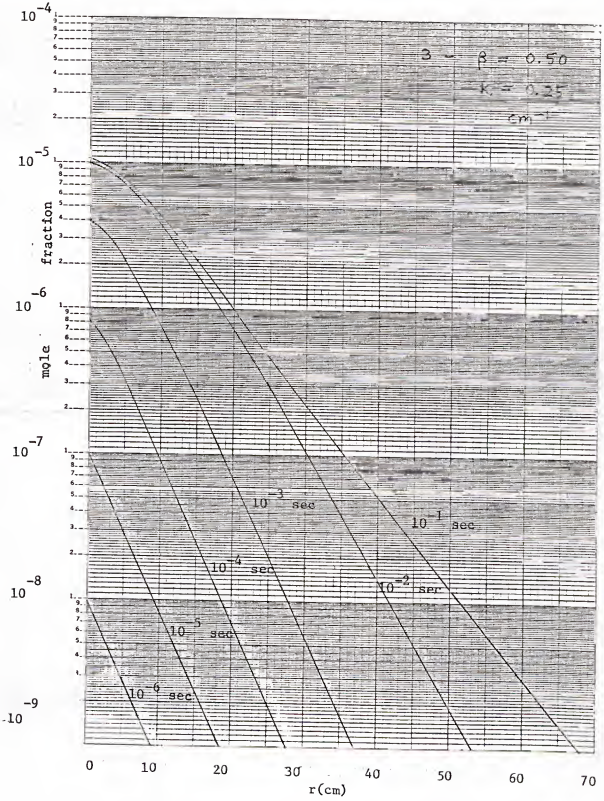


Figure 3.10. Time sequence of radial profiles for single body decay, $\beta = .50\ cm^{-1}$, $\kappa = .25\ cm^{-1}$.

.0021 sec and .00021 sec, respectively. The diffusion convergence time $\tau_D = 1/D\beta^2 = .0088$ sec. These four cases then give one slow chemistry, one with chemical reaction time equal to diffusion convergence time, and two with fast chemistry.

Making the transformation $C = G/r$, and considering only the steady state limit, Eq. (3.39) becomes

$$G'' - \frac{2k}{D}\frac{G^2}{r} + Bre^{-\beta r} = 0 \tag{3.40}$$

We may define an inverse length κ associated with k/D but in a different way than in the single body case. We may ask that κ^2 be replaced by κ^4 reflecting the number of bodies. We may allow it to become a coefficient of the second term by admitting a compensating coefficient. Finally, we may look somewhere else for analogies--namely, we may compare the pure diffusion steady state peak $(A/D\beta^2 = B/\beta^2)$ with the pure kinetic steady state limit $(\sqrt{A/2k})$. This suggests that we define $\kappa = \sqrt[4]{2kA/D^2} = \sqrt[4]{2kB/D}$ so that $B/\kappa^2 = \sqrt{A/2k}$. Equation (3.40) then becomes

$$G'' - \frac{\kappa^4 G^2}{Br} + Bre^{-\beta r} = 0 \tag{3.41}$$

This is all very well and good, but what has it gained us? We look at Fig. 3.11 where the time dependence of the solution at r=0 is plotted for the four cases listed above and for pure diffusion for comparison. For the four values of k listed above, $\kappa = .16$, .25, .51 and 1.6. Here now is the rest of the explanation for the choice of the values of k: we find that by defining κ as we did, so that the forms for steady

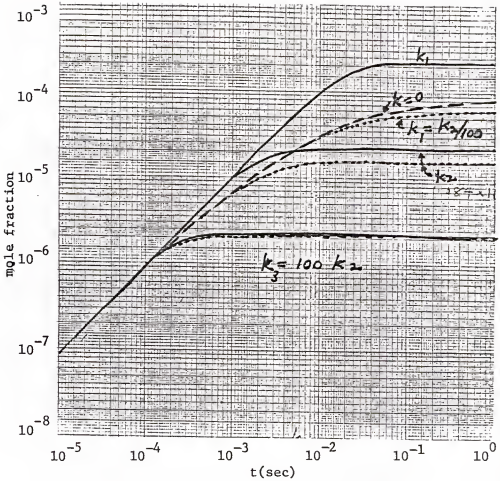


Figure 3.11. Time course for two body single species decay at r = 0. Three cases shown. Corresponding pure kinetic cases and pure diffusion shown for comparison.

state pure diffusion peak value and steady state pure kinetic steady state peak value are analogous, a 'characteristic diffusion time', $1/D\beta^2$ is indicated by analogy: $\beta = \kappa \Rightarrow \tau_d = \tau_c$. Noting the values of the steady state limits at r=0 for the assorted diffusion kinetic cases, we find that, to an average accuracy of < 10%, this limit is given by $C = B/(\beta^2 + \kappa^2)$. We may refer to the case $\kappa \ll \beta$ ($\tau_c \gg \tau_d$) as weak, slow or late chemistry, and to the case $\kappa \gg \beta$ ($\tau_c \ll \tau_d$) as strong, fast or early chemistry.

The time evolutions of profiles for the first, third and fourth cases listed above are plotted in Figs. 3.12-14. The steady state profiles of all four cases along with the steady state profile for pure diffusion are plotted in Fig. 3.15. A striking and very interesting array of patterns meets us here. Looking at the time sequences of profiles, we observe that as the chemistry becomes stronger, the evolution of the steady state profile resembles the stripping away from an irreducible core of more and more covering.

What is happening is this. In the core, as the chemistry becomes faster, it seats a steady state profile long before diffusion can have an effect, resulting in a purely local chemical effect. Thus in the core the effect of the diffusion term drops off, leaving a local balance between destruction term and source term.

In the limb the effect of the short range source term dies away. Without chemistry the pure diffusion 1/r limit would take place, reflecting only diffusion. With chemistry, a balance is set up between diffusion and chemical destruction:

$$G'' - \frac{2k}{D}\frac{G^2}{r} = 0 \text{ or } G'' - \frac{\kappa^4}{B}\frac{G^2}{r} = 0 \qquad (3.42)$$

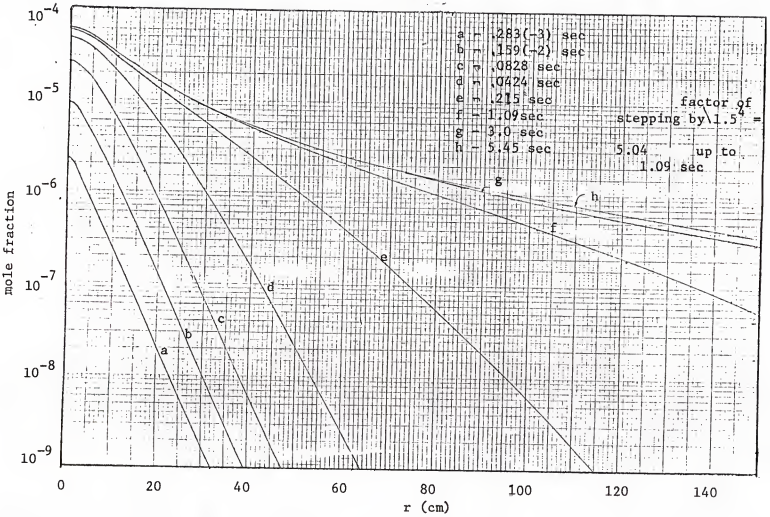


Figure 3.12. Time sequence of radial profiles for two body single species decay, $\beta = .25\ cm^{-1}$. $\kappa = .16\ cm^{-1}$.

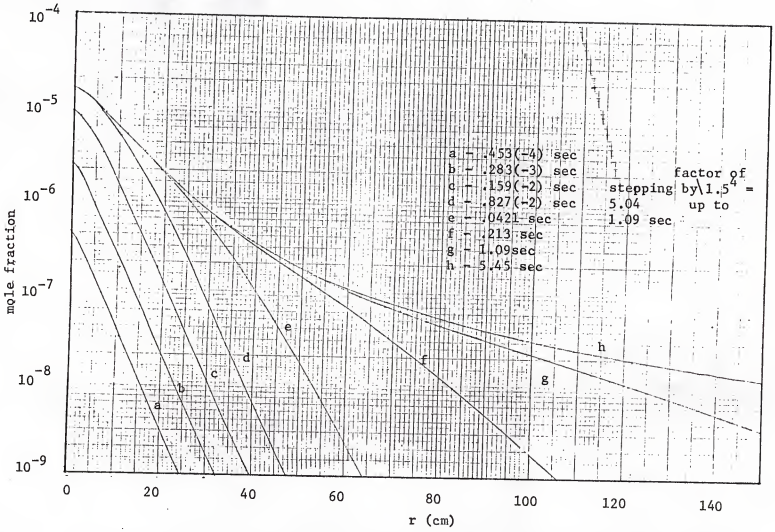


Figure 3.13. Time sequence of radial profiles for two body single species decay. β = .25 cm^{-1}. κ .51 cm^{-1}.

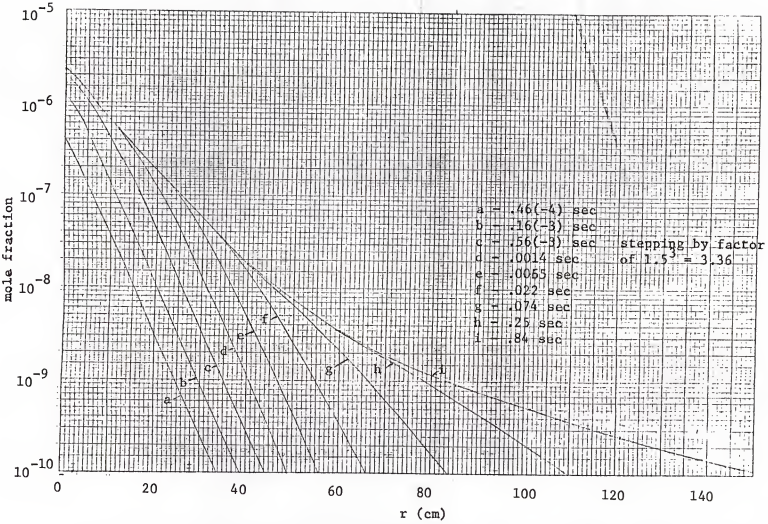


Figure 3.14. Time sequence of radial profiles for two body single species decay. $\beta = .25\ cm^{-1}$. $\kappa = 1.6\ cm^{-1}$.

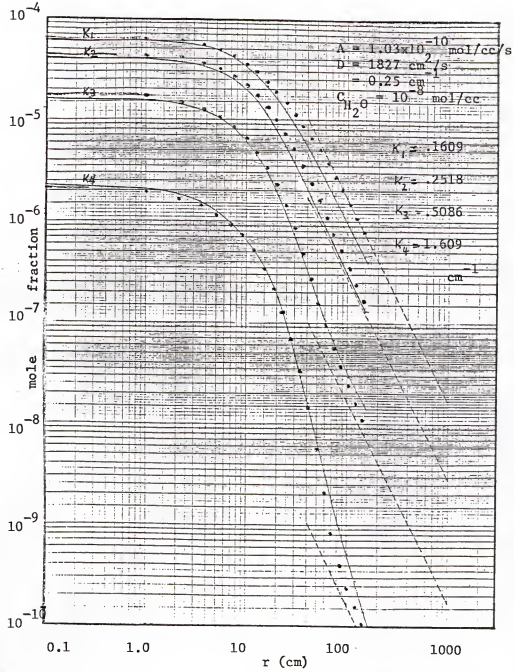


Figure 3.15. Steady state profiles for two body single species decay: β = .25 cm^{-1}. κ = .16 cm^{-1}, .25 cm^{-1}, .51 cm^{-1} and 1.6 cm^{-1}. Overlaid by fit obtained in Appendix D.

This asymptotically limiting form of the equation is solved by the power law form, $G = 2B/\kappa^4 r = D/kr$ (wherefore $C = 2B/\kappa^4 r^2 = D/kr^2$), which is independent of A, the scaling of the source. This invariance is a result of the nonlinear dependence on concentration of the diffusion-kinetic balance. Looking to Fig. 3.15 we note that the solution as calculated numerically is indeed approaching the asymptote, except for the weakest chemistry case, in which a 50% discrepancy appears. This has not yet been explained and may be a numerical artifact.

Proceeding from these asymptotic trends in κ/β and r, it is possible to construct an analytic form which splines them together over the entire range of κ/β. This has been done, and the derivation and form are presented in Appendix D. Resultant values are overlaid on the true values in Fig. 3.15. Agreement is very good. With a little effort it should also prove possible to find a suitable analytic spline which patches together early and later time asymptotic limits.

Two Species Two Body Decay--Specific Example

In the case of two body decay coupling two distinct species, two new degrees of freedom are introduced: (1) $y_1 \neq y_2$, and (2) $D_1 \neq D_2$. We consider the reaction

$$H + OH + M \rightarrow H_2O + M \tag{3.43}$$

with T = 400 K, n = 1.84×10^{19} #/cc (p = 1 atm). The source terms, y_H and y_{OH}, are taken to be the post-recombination spatial yields obtaining for a 1 keV electron beam. These stand in the ratio, $y_1/y_2 = 1.1$. The diffusion coefficients, found from Table 6.1, stand in the ratio, $D_1/D_2 = 3.5$. Curiously enough, as we shall see below, the more powerful effect is from the differential in source term.

Three injection rates are considered: $I = I_1 = 3.67 \times 10^{10}$ #/sec, $I = 100\ I_1$, and $I = 10^4 \times I_1$. Reaction times are 1.3×10^{-5} sec, 1.3×10^{-6} sec, and 1.3×10^{-7} sec, respectively. Diffusion convergence time is 1.3×10^{-6} sec. Thus, $\tau_c = 10\tau_d$, $\tau_c = \tau_d$, and $\tau_c = \tau_d/10$, or equivalently, $\beta^2 = 10\kappa^2$, $\beta^2 = \kappa^2$ and $\beta^2 = \kappa^2/10$, respectively. We thus have one representative case each of slow, borderline and fast chemistry. The problem is abstracted from the three cases at one atmosphere pressure, T = 400 K, and for E_o = 1 keV considered in Chapter VI. Although we did not consider the evolution of the concentration of product species in the previous section, we do so here, labelling product H_2O separately from the medium.

Time course of the system at r = 0 is plotted for these three cases in Figs. 3.16-18. Time sequences of radial profiles are plotted in

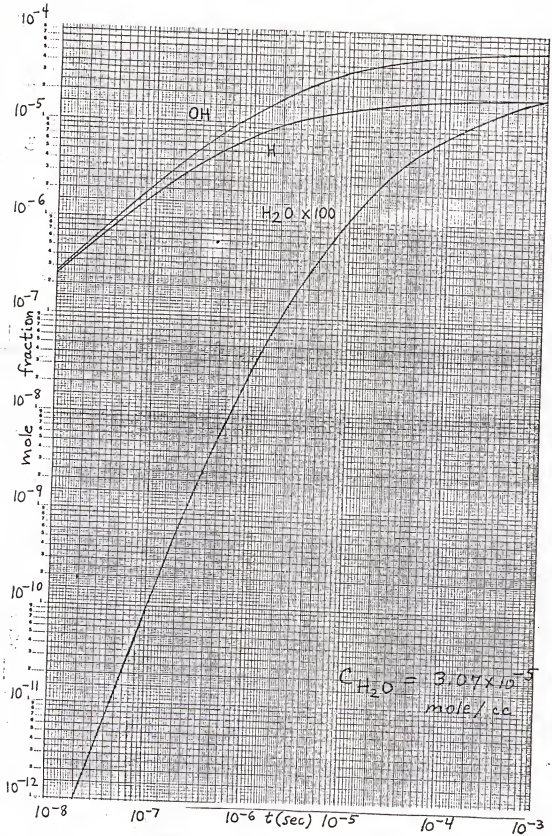


Figure 3.16. Time course at r = 0 for $H + OH + M \rightarrow H_2O + M$. Slow chemistry case. Compare Figure 6.6.

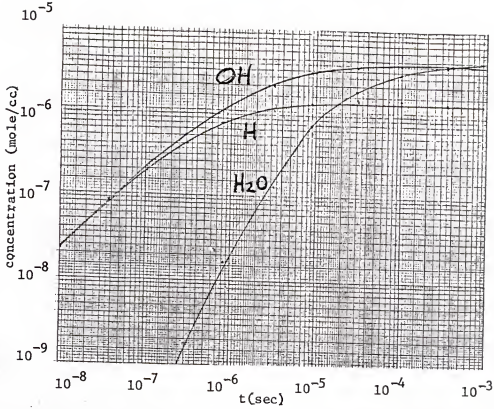


Figure 3.17. Time course at r = 0 for $H + OH + M \rightarrow H_2O + M$. Borderline chemistry case. Compare Figure 6.8.

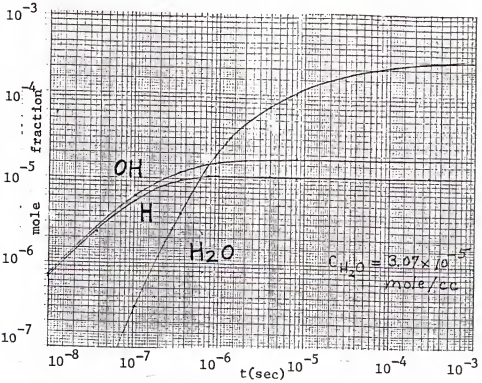


Figure 3.18. Time course at r = 0 for $H + OH + M \rightarrow H_2O + M$. Fast chemistry case. Compare Figure 6.10.

Figs. 3.19a-c, 3.20a-c, and 3.21a-c. Let us consider the first case, the slow chemistry case (see the first time plot and the first group of radial profile time sequences).

The Slow Chemistry Case

In the slow chemistry case diffusion shaped profiles have converged before reaction time at center is reached. From this point on, it becomes relevant to compare with the reaction time for initial concentrations, thinking in terms of reinitialized time. The reaction time follows from Eqs. 3.6 and 3.9 and is given by Eq. (4.11), and, substituting values of concentrations and reaction rate coefficient, we obtain $\tau_c = 2.4 \times 10^{-4}$ sec. Why then is product H_2O concentration at $r = 0$ is still not completely converged at $t = 10^{-3}$ sec? There are two reasons: (1) convergence is more gradual in the initial pulse case (compare Figs. 3.1 and 3.2), and (2) the source term of product H_2O continues to spread outward after it has converged in the center. H_2O produced in the limb diffuses towards the center as well as outward. As a result the product H_2O concentration at the center continues to increase, prolonging the convergence.

Since the time courses of the reactant concentrations are those for pure diffusion, for which we have an accurate analytic representation, we may calculate the time course of the product concentration by means of the Green's function integral. Results are overlaid in Fig. 3.19c. (To illustrate the quality of the fit to the diffusion time courses, the pure diffusion fit is overlaid in Figs. 3.19a and b. The agreement of the calculated product concentration predicted on the basis of the

Figure 3.19. Time sequence of radial profiles for (a) H, (b) OH and (c) H_2O in the slow chemistry case. Overlaid by pure diffusion fit in (a) and (b) and by Green's function integral calculated value in (c) based on pure diffusion fits in (a) and (b).

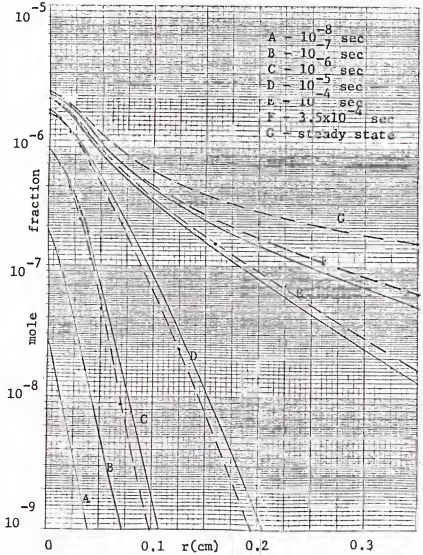


Figure 3.19 (a)

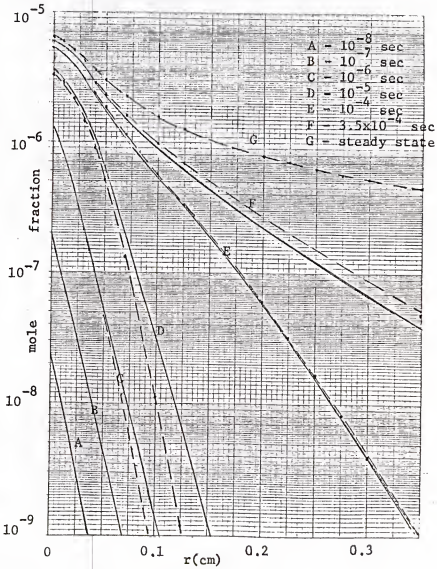


Figure 3.19 (b)

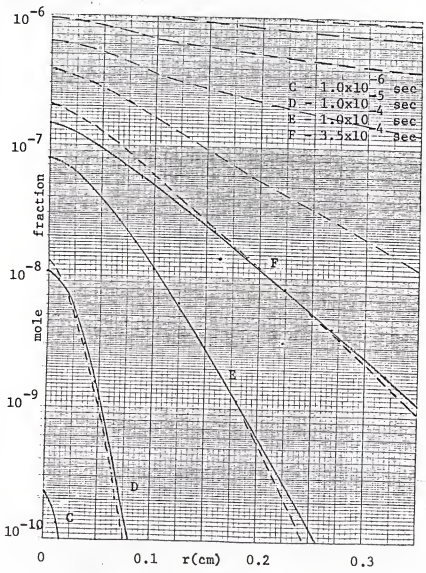

10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
mole fraction
C - 1.0×10^{-6} sec
D - 1.0×10^{-5} sec
E - 1.0×10^{-4} sec
F - 3.5×10^{-4} sec
C
D
E
F
0
0.1
r(cm)
0.2
0.3

Figure 3.19 (c)

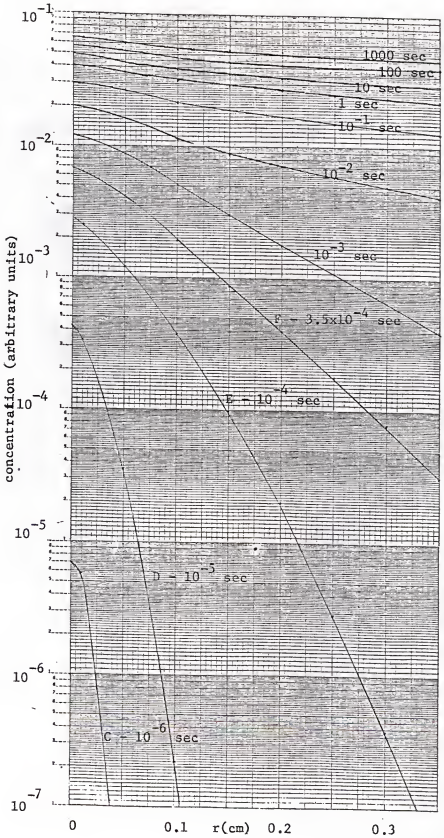

concentration (arbitrary units)
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
1000 sec
100 sec
10 sec
1 sec
10^{-1} sec
10^{-2} sec
10^{-3} sec
E - 3.5×10^{-4} sec
F - 10^{-4} sec
D - 10^{-5} sec
C - 10^{-6} sec
0
0.1
r(cm)
0.2
0.3

Figure 3.19 (c')

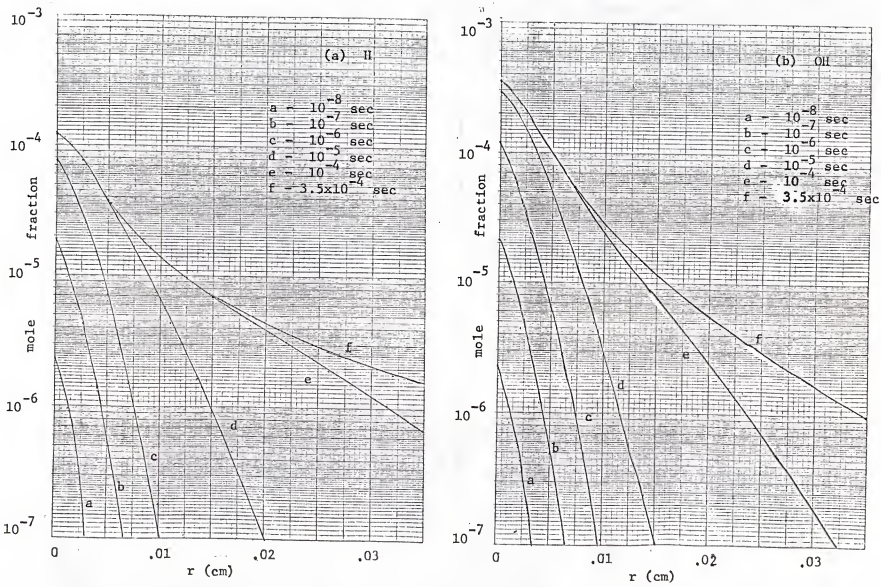


Figure 3.20. Time sequence of radial profiles for (a) H, (b) OH.

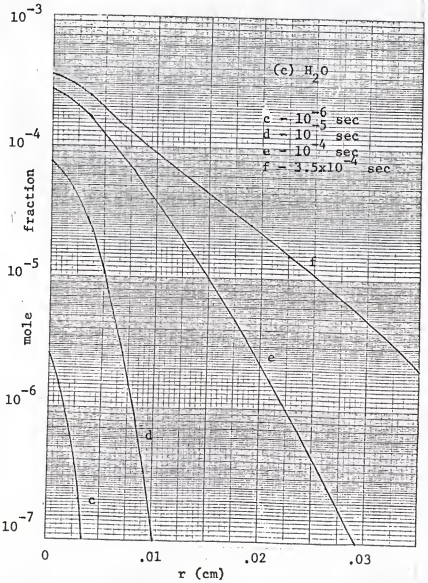


Figure 3.20. Time sequence of radial profiles for (c) H_2) in the borderline chemistry case.

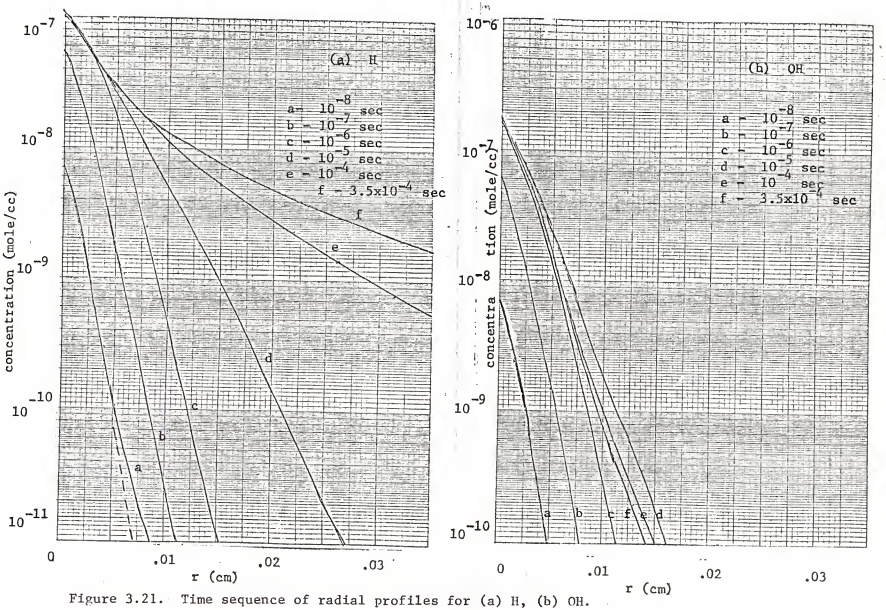


Figure 3.21. Time sequence of radial profiles for (a) H, (b) OH.

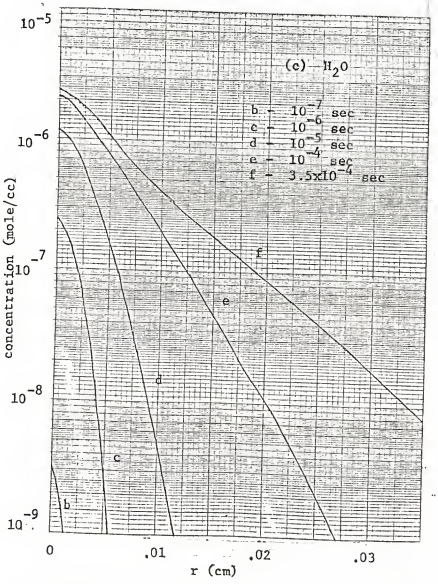


Figure 3.21. Time sequence of radial profiles for (c) H_2O in the fast chemistry case.

fitted reactant concentrations is remarkably good. With it we can predict the time course out to very distant times out to which it would be impractical to calculate using the marching step code. Results at these later times are also plotted in Fig. 3.19c.

Looking at the overlay in Fig. 3.19c, or in Fig. 3.19c' where it is taken out to much longer times, it becomes apparent, assuming this numerical integral is correct, that the growth becomes logarithmic.

This result is easily confirmed analytically. The source term is proportional to $1/r^2$ in the limbs, cancelling the volume element scale factor. The effective upper limit for r is $\sqrt{4D\tau}$. Partial cancellation of the $(4D\tau)^{3/2}$ in the denominator of the τ-integral then yields the logarithmic result. The numerical result is, therefore, correct.

Borderline and Fast Chemistry Cases

We next consider the two other cases of borderline chemistry and fast chemistry. In contrast with the sequence of cases in the single species case (previous section) where the reaction rate coefficient was varied while the source term, y, remained fixed, here--in a physically realistic context--the rate coefficient remains fixed (for fixed density the effective two body rate coefficient implied by the three body coefficient is fixed), while the source term is varied. Comparison is therefore aided by scaling concentrations to source term. In this context it is relevant to consider Fig. 3.11 where diffusion kinetic time courses at r=0 are compared with the corresponding pure kinetic courses and the corresponding pure diffusion time course for the single species case.

Although it would be informative to similarly graph corresponding time courses together on one graph here, we can derive the essence of this information from Table 3.1 in which steady state peak values are compared.

In the borderline case, the peak levels of both reactant species are diminished by the same relative amounts. Both profiles exhibit the stronger convergence to steady state near the peak characteristic of increasing chemical effect. The fall offs of both profiles have become steeper by a small amount, somewhat more for OH than for H, even relative to its extent.

In the fast chemistry case, the OH peak level is decreased by twice as much as is the H peak, bringing them closer to their source term ratio, 1.1:1. This increased localization reflects the greater speed of the chemistry outpacing the slower diffusion (nonlocalizing effect).

The H fall off becomes even broader, while the OH fall off becomes extremely steep, in fact, essentially exponential fall off. The greater diffusivity of H is not the source of this effect. The differential in the source terms is. Recall the results for two species two body decay for unequal source terms in the pure kinetic case. In the steady state limit the minority species decays to zero while the majority species then grows at the rate of the difference of their source terms. In the diffusion kinetic case, diffusion braking sets a limit on the scavenging strength of the majority species, and, as a result, a nonzero fraction of the minority species escaped destruction, while the majority species enjoys a pure diffusion limit in the limb.

TABLE 3.1
Comparison of Steady State Peak Concentrations

(first entry is mole fraction; second entry is mole fraction normalized to injection rate of slow chemistry case; third entry is this quantity normalized to slow chemistry mole fraction)

	H	OH
slow chemistry	2.0(-6) 2.0(-6) 1	5.6(-6) 5.6(-6) 1
borderline chem.	1.2(-4) 1.2(-6) .6	3.6(-4) 3.6(-6) .6
fast chemistry	4.0(-3) 4.0(-7) .2	6.0(-3) 6.0(-7) .1

The gradual 1/r fall off of the majority species has about the same effect as a constant level and the steady state limit profile of the minority species is essentially exponential, mimicking single-body decay.

Fast Chemistry with Reactant Yield Rates Interchanged

In order to demonstrate conclusively that the effect seen here is due to the 10% difference in the yield rates, rather than to the large difference in the diffusion constants, the same system was recalculated with the yield rates interchanged. The time plot is given in Fig. 3.22, and the profiles are given in Fig. 3.23. It can be seen at once that the differential in the yield rates is the source of the effect. Here the OH enjoys the pure diffusion limit in the limb, while the H is held down to an essentially exponential fall off. The strange behavior in the later time H profiles in the limb may be a numerical artifact or partly so. This question could be resolved by increasing the number of radial grid points and extending the edge point outward, and replacing the Simpson rule interpolation by cubic interpolation (see Appendix B).

We note that the H_2O profiles are only minimally perturbed by the interchange in yield rates. This makes sense since the H_2O production rate is proportional to the product of the H and OH concentration levels. Thus, to start with, at early times before diffusion has an effect, nothing is changed for H_2O production. At later times it can be seen from the profile plots that the bulk of newly created H and OH go into H_2O production; therefore, there is little change here either.

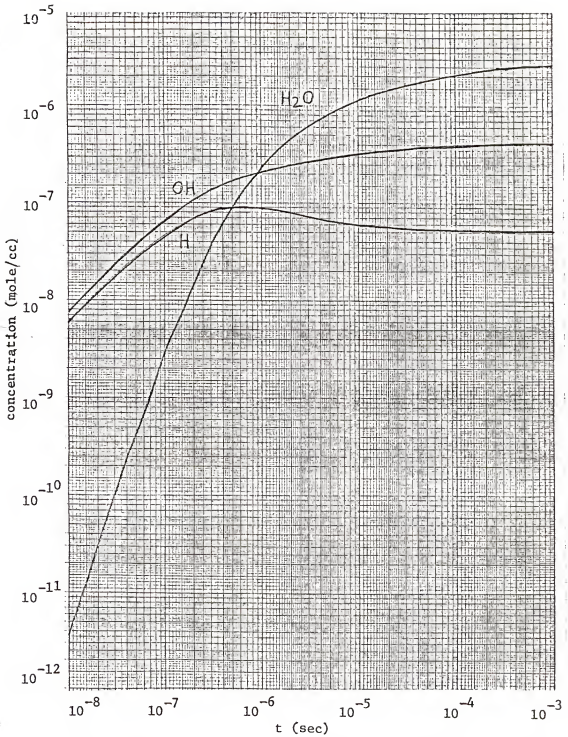


Figure 3.22. Time course at r = 0 for H + OH + M → H_2O + M. Fast chemistry case. H and OH yield rates reversed. Compare with Figure 3.15.

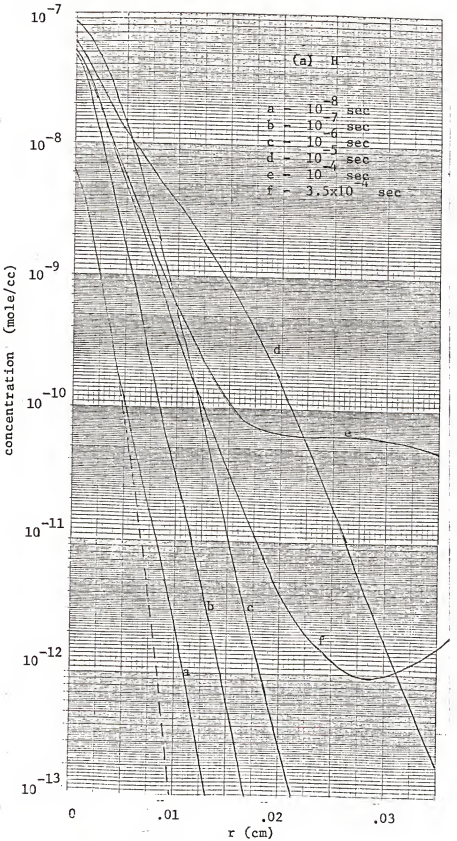


Figure 3.23. Time sequence of radial profiles for (a) H.

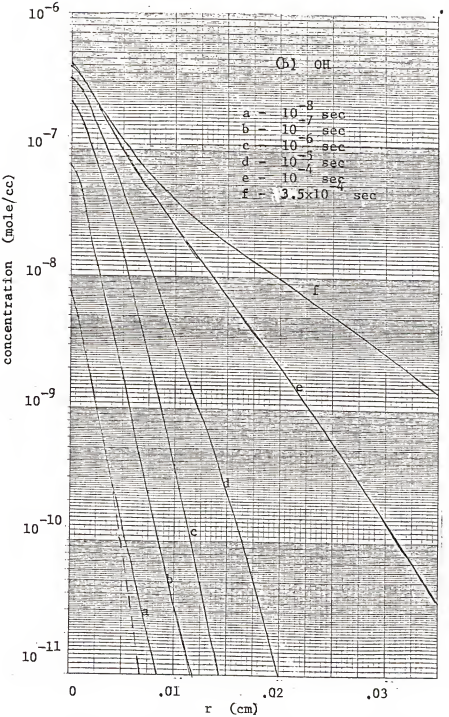


Figure 3.23. Time sequence of radial profiles for (b) OH.

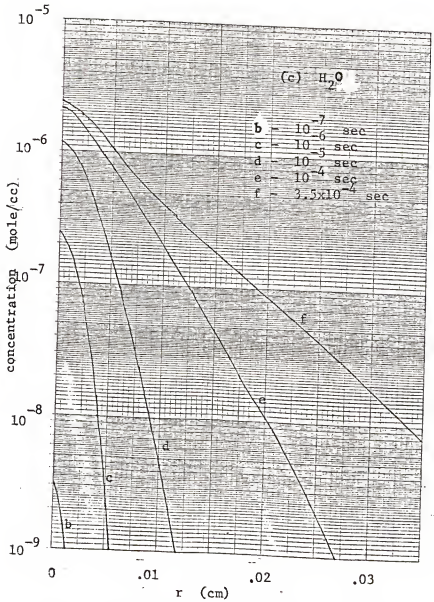


Figure 3.23. Time sequence of radial profiles for (c) H_2O in the reversed fast chemistry case. Compare with Figure 3.18.

We note, finally, the still lower level of H radical at r=0 in the steady state limit as a result of the interchange of yield rates. Whereas it was lower before because of its greater diffusivity sending it out to the limb, it is still lower here as a result of the loss of advantage in source term. The hump in the time course at r=0 and the broad swing out and back in the profile reflect further this association of high diffusivity with disadvantage in yield rate. In the intermediate time frame of this swing, the more diffusive minority species (H) has a greater survival rate in the limb where the more slowly moving majority species (OH) has not yet reached. This phase comes to an end, however, in a delayed outward sweep of OH chasing after this escaped prey. The pinched off bubble of H moving outward ahead of the OH may therefore be at least partly real.

Where We Go From Here

This, finally, is a good point at which to pause for a moment and take stock before proceeding. We have laid out the mathematical formulae of simple kinetics of one and two body decay for both initial pulse and continuous steady pulse source terms, for both one species and two species reactive systems. We have calculated the complete time dependence of pure diffusion for spherical geometry, and characterized it in sufficient detail to aid us in our diffusion kinetic work.

Since the overall features of both diffusion and kinetics are intuitively straight forward, the important benefit of this work was quantitative identification of reaction times and diffusion convergence time.

With these basic results at our disposal, we then went on to consider diffusion kinetics of one and two body decay. More attention was paid to two body decay. However, effective one body decay through reaction with the medium (H_2O) does occur in both the ion and the neutral reactive systems.

Two body decay was first treated in the simpler context of single species. Analytic asymptotic limits were identified. The interplay of diffusion and kinetics was clearly discerned. The two species case was considered in the specific physical context of the reaction, $H + OH + M \rightarrow H_2O + M$, for realistic radiological inputs, in fact for one of the density-temperature-incident energy configurations which will be considered in Chapter VI, so that isolation of effect is possible.

What remains to be done is as follows: 1. The instantaneous treatment of the ion reactions must be put in place before we can proceed to the neutral reaction set operating by itself. 2. The kinetics of the neutral reaction set are to be identified. Since we view diffusion kinetics--in the context of the type of problem considered here--as diffusion limitation or modification of kinetics, we need kinetics to modify. Diffusion kinetics of the full neutral reaction set. Here we tie back in to the spatial yields, and finally, into their energy dependence, and therewith the energy dependence of the diffusion kinetics.

CHAPTER IV
ION REACTIONS

The ion reactions divide into three categories: (1) ion-neutral reactions, for which only those in which H_2O is the neutral species are of any consequence due to concentration, (2) hydration of the proton, which as we will see below has negligible stoichiometric effect, and (3) proton-electron recombination.

In his Ph. D. thesis (1983) Rio has compiled the predominant ion reactions (and associated reaction rates) which take place in water vapor subjected to electron bombardment (at low temperatures, i. e., ca. 200 - 450 K). We adopt this reaction set here. Reaction 43 ($H_2O^+ + H_2 \rightarrow H_3O^+ + H$) is omitted for the reason mentioned above. These reactions and reaction rates are given in Table 4.1. The sources of these reactions and reaction rates are: Huntress (1973) and Ferguson (1973) for the ion-neutral reactions; Good et al. (1970) for the ion clustering reactions; and Leu et al. (1973) for the recombination reactions.

The neutral reactions and reaction rates are taken from a recent combustion oriented compilation of Westbrook (1981), and are given in Table 4.2. These are the same as used by Rio, and have been implemented in previous combustion (and radiolysis) related work in this group (Green et al., 1983; Pamidimukkala et al., 1983).

It is a well known fact that the ion reactions proceed much faster than the reactions between neutrals for typical medium densities and injection rates. Taking typical concentrations into account, a quick

TABLE 4.1
Reactions and Reaction Rates for the Ions

	Reaction		Reaction Rate Coefficient at ca. 300-400 K (cc-mole-sec)
a	$H_2O^+ + H_2O$	$\rightarrow H_3O^+ + OH$	1.14(15)
b	$OH^+ + H_2O$	$\rightarrow H_2O^+ + OH$	3.49(14)
c	$OH^+ + H_2O$	$\rightarrow H_3O^+ + O$	2.83(14)
d	$H^+ + H_2O$	$\rightarrow H_2O^+ + H$	4.94(15)
e	$H_3O^+ + H_2O + M$	$\rightarrow H^+(H_2O)_2 + M$	1.23(21)
f	$H^+(H_2O)_2 + H_2O + M$	$\rightarrow H^+(H_2O)_3 + M$	8.34(20)
g	$H^+(H_2O)_2 + e^-$	$\rightarrow H + H_2O + H_2O$	1.63(18)
h	$H^+(H_2O)_3 + e^-$	$\rightarrow H + H_2O + H_2O + H_2O$	2.77(18)
i	$H_3O^+ + e^-$	$\rightarrow H + H_2O$	7.83(17)
j	$H_3O^+ + e^-$	$\rightarrow H + H + OH$	<<7.83(17)

TABLE 4.2
Reactions and Reaction Rates for the Neutrals

(Reaction rate coefficients are in cc-mole-sec units.)

Reaction	Reaction Rate Coefficient at T = 300 K	400 K
1f $H + O_2 \rightarrow O + OH$	1.09(2)	1.24(5)
1b $H + O_2 \leftarrow O + OH$	4.73(12)	6.29(12)
2f $H_2 + O \rightarrow H + OH$	1.76(6)	9.95(7)
2b $H_2 + O \leftarrow H + OH$	2.16(7)	5.30(8)
3f $H_2O + O \rightarrow OH + OH$	1.45	3.19(3)
3b $H_2O + O \leftarrow OH + OH$	5.00(11)	7.91(11)
4f $H_2O + H \rightarrow H_2 + OH$	1.55(-1)	7.73(2)
4b $H_2O + H \leftarrow H_2 + OH$	3.87(9)	3.36(10)
5f $H_2O_2 + OH \rightarrow H_2O + HO_2$	4.88(11)	1.04(12)
5b $H_2O_2 + OH \leftarrow H_2O + HO_2$	3.64(-11)	3.43(-5)
6f $H_2O + M \rightarrow H + OH + M$	7.00(-60)	9.00(-42)
6b $H_2O + M \leftarrow H + OH + M$	1.57(18)	8.81(17)
7f $H + O_2 + M \rightarrow HO_2 + M$	8.88(15)	5.84(15)
7b $H + O_2 + M \leftarrow HO_2 + M$	8.30(-19)	1.90(-10)
8f $HO_2 + O \rightarrow OH + O_2$	9.36(12)	1.42(13)
8b $HO_2 + O \leftarrow OH + O_2$	3.68(-28)	7.54(-18)

9f	$HO_2 + H \rightarrow OH + OH$	1.04(13)	2.30(13)
9b	$HO_2 + H \leftarrow OH + OH$	7.32(-17)	1.47(-9)
10f	$HO_2 + H \rightarrow H_2 + O_2$	7.76(12)	1.04(13)
10b	$HO_2 + H \leftarrow H_2 + O_2$	4.26(-29)	1.43(-18)
11f	$HO_2 + OH \rightarrow H_2O + O_2$	9.36(12)	1.42(13)
11b	$HO_2 + OH \leftarrow H_2O + O_2$	9.74(-40)	2.76(-26)
12f	$H_2O_2 + O_2 \rightarrow HO_2 + HO_2$	3.42(-18)	2.00(-10)
12b	$H_2O_2 + O_2 \leftarrow HO_2 + HO_2$	1.87(12)	2.84(12)
13f	$H_2O_2 + M \rightarrow OH + OH + M$	8.52(-17)	1.65(-8)
13b	$H_2O_2 + M \leftarrow OH + OH + M$	4.51(18)	5.38(17)
14f	$H_2O_2 + H \rightarrow HO_2 + H_2$	3.15(9)	1.51(10)
14b	$H_2O_2 + H \leftarrow HO_2 + H_2$	1.72(-2)	43.8
15f	$O + H + M \rightarrow OH + M$	1.00(16)	1.00(16)
15b	$O + H + M \leftarrow OH + M$	0.	4.20(-40)
16f	$O_2 + M \rightarrow O + O + M$	0.	7.40(-48)
16b	$O_2 + M \leftarrow O + O + M$	9.47(14)	8.74(14)
17f	$H_2 + M \rightarrow H + H + M$	2.50(-56)	7.66(-39)
17b	$H_2 + M \leftarrow H + H + M$	3.02(15)	3.02(15)

glance at the reaction rates in Tables 4.1 and 4.2 makes this clear. In order to properly compare, typical concentrations must be taken into account. In the interest of thoroughness it would be advantageous to compare over a representative grid in medium density and injection rate. This is done in the last section of this chapter with follow-up in the last section of the following chapter.

Rather than just look at isolated reaction rates, it is much more informative to calculate the evolution of the full kinetic system of ions and neutrals in order to identify the characteristic trends of the ion regime and of the separation of time scales of the two systems. For this purpose both the initial pulse case and the continuous pulse case are of interest. It would be useful to perform such kinetic calculations over the above mentioned representative grid in medium density and injection rate. To this purpose the code DIFKIN, written to calculate diffusion kinetics or pure kinetics, could be used. However, a pre-existing kinetic code written by Rio (Ph. D. thesis, 1983) based on a the Gear method (Hindmarsh, 1974) has already proved useful to this purpose, as demonstrated by the initial pulse calculation presented in Rio (Ph. D. thesis, 1983, Fig. 3.1) and reproduced here in Fig. 4.1. This kinetic plot is extremely informative and we shall now discuss it.

The H_2O concentration is 1×10^{-7} moles/cc. The initial concentrations of the radiological deposition products are apparent from the plot. As stated by Rio, these concentrations were chosen to be proportional to the initial radiological yields. These proportions are essentially constant with respect to E_o as a result of the essentially constancy of the g-values (see Chapter II).

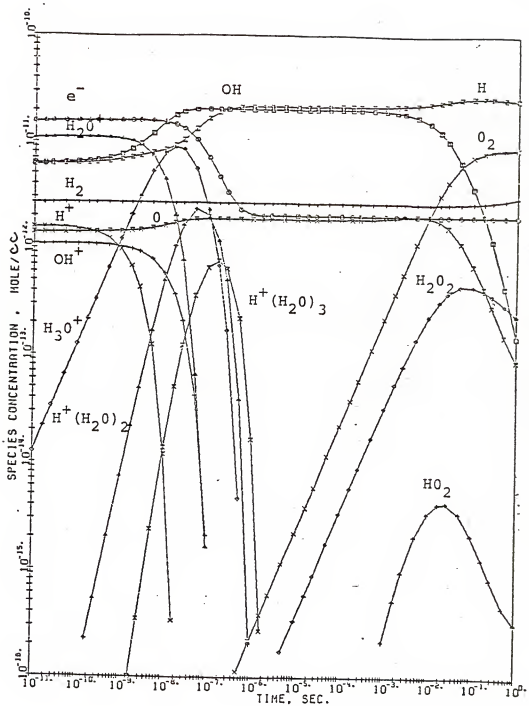


Figure 4.1. Kinetic time course of full ion-neutral system for initial pulse, (Rio, Ph.D. thesis, 1983).

Inspection of this plot reveals that proton transfer from H_2O^+, the dominant primary ionic species, to H_2O, is well underway by 10^{-8} sec. Specifically, the H_2O^+ concentration has fallen by a factor of about 1/e at this time. H_3O^+ peaks shortly after that, with $H^+(H_2O)_2$ peaking shortly after it, and $H^+(H_2O)_3$ shortly after it, spread over the interval 2×10^{-8} sec $< t <$ 2×10^{-7} sec. Recombination gets underway at about 2×10^{-8} sec and is essentially complete by 5×10^{-7} sec. The neutral reactions do not become critical until after 1×10^{-3} sec. Thus, the ion reactions are well separated from the neutral reactions in time--by more than three, almost four orders of magnitude.

It may be noted in passing that electron recombination with the primary yield ions occurs, but at a rate negligible in comparison with the rate of their reaction with the much more numerous H_2O molecules.

Inferring from the comfortable separation of time scales between the ion reactions and the neutral reactions, we may conclude that for a wide range of medium densities and injection rates that this separation would maintain. Where it may begin to break down should be at higher densities, where the enhanced reaction rate of the three body radical recombination reactions would begin to push the onset of neutral activity backward in time. Such a calculation at liquid density, for example, should be made to span the interval so that we may speak with some confidence of this.

Reduced Reaction Set

Because the ion reactions are all one-way, and a nondepleting regime is assumed, ruling out feedback loops via reactions of the ions

with neutrals other than H_2O, the ion reactions constitute a feedforward system. Reactions b and d (electron transfer) feed into reaction c (proton transfer) which parallels reaction a (proton transfer). The end point of these reactions of the ions with H_2O is the hydronium ion, H_3O^+.

Noting the increase in the recombination reaction rates with increasing level of hydration, it follows that the effect of the multiple hydration (reactions e and f) is to shorten the time the proton remains imrecombined. This trend in reaction rate, therefore in reaction cross section is apparently due to a diffusion of positive charge over a greater volume via polarization.

The end step, electron-proton recombination splinters off these associated H_2O molecules, and finalizes the production of H. Reaction j is energetically unfavored, and so can be neglected. As a result, the multiple hydration reactions have negligible stoichiometric effect.

From the above analysis we may predict the post-recombination concentrations in terms of the initial concentrations following an initial pulse of the electron beam, and post-recombination yield rates in terms of "initial" yield rates for a continuous beam, assuming the one other important point which we will get to momentarily, the separation in time scales of the ion reactions from the neutral reactions. For the moment this will be assumed. Let us first consider the case of an initial pulse. We first define a quantity f which defaults to 1 if the electrons outnumber the ions, and which otherwise refects the electron deficit. Formally, we may write

$$f = r(1-\theta(r-1)) + \theta(r-1) \qquad (4.1)$$

where

$$r = (e^-)/[(H^+) + (OH^+) + (H_2O^+)] \tag{4.2}$$

and θ is the Heaviside step function. The post-recombination concentrations in terms of the initial concentrations are then given by

$$[H] = (H) + (H^+) + f[(OH^+) + (H^+) + (H_2O^+)] \tag{4.3a}$$

$$[H_2] = (H_2) \tag{4.3b}$$

$$[OH] = (OH) + (2k_b/(k_b+k_c))(OH^+) + (H^+) + (H_2O^+) \tag{4.3c}$$

$$[O] = (O) + (k_c/(k_b+k_c))(OH^+) \tag{4.3d}$$

$$[e^-] = (e^-) - f[(OH^+) + (H^+) + (H_2O^+)] \tag{4.3e}$$

$$[H^+] = [OH^+] = [H_2O^+] = 0 \tag{4.3f}$$

$$[H^+(H_2O)_n] = (1-f)[(OH^+) + (H^+) + (H_2O^+)] \tag{4.3g}$$

where the parentheses indicate initial concentrations, and brackets indicate post-recombination concentrations. The various levels of clustering of the hydrated proton are indicated collectively by $H^+(H_2O)_n$. By post-recombination is meant for times up until the neutral reactions get underway.

When we think of Equations (4.3a-g) in the yield rate sense, it is necessary to include the yield rate for H_2O, which follow from mass conservation:

$$(H_2O) = -(OH) - (O) - (OH^+) - (H_2O^+) \tag{4.4a}$$

$$= -\left[(H_2) + (H_2O^+)\right] - \frac{1}{2}\left[(H) + (H^+) + (OH) + (OH^+)\right]. \tag{4.4b}$$

In the post-recombination phase additional H_2O molecules have been broken up as a result of electron transfer from H_2O to H^+ and OH^+ (reactions b and d) to yield H_2O^+ which then loses a proton to H_2O (reaction a) to yield OH and H_3O^+. In all the other reactions H_2O merely serves as a catalyst to reactions which do not break up H_2O molecules. It follows that

$$[H_2O] = (H_2O) - (H^+) - \frac{k_b}{k_b + k_c}(OH^+) \tag{4.5}$$

independent of f.

We may check our predictions for the post-recombination concentration levels against the results of Rio's code, both for the case of initial pulse, and for the case of a steady beam, which integrates out from the initial pulse case--as far as the ion reactions are concerned. We find that our predictions are borne out to four significant figures. This is not too surprising, since all we were calculating were final states, or asymptotic limits.

From the above it is clear that all concentrations of interest except for the individual breakdown of the collectively defined hydrated proton, and the concentrations of the unreacted primary ions, which are minuscule, can be calculated solely on the basis of neutral chemistry and electron-proton recombination.

If the electron yield is everywhere greater than the ion yield, then the problem reduces to one of only neutral chemistry. If this is not the case, then the mobility of the electron comes into play.

Charge Separation and Electron Mobility

The charge separation which is present already in the initial deposition, in greater or lesser degree, depending on incident energy creates an electrostatic force field which influences the motion of the electron and, to a lesser extent because of their far greater masses, the motion of the ions. Specifically, it gives rise to a drift velocity, $\vec{v}$, given by $\vec{v} = \mu\vec{E}$ where μ is defined as the mobility coefficient and is given by $\mu = (e/m)\nu_c$ where ν_c is the frequency of collisions (Allis, 1956; Brown, 1958).

A convective term is thereby introduced into the diffusion kinetic equation for the electron (the convective term for the positive ions can be relatively ignored):

$$\frac{\partial c_e}{\partial t} - \mu\vec{E}\cdot\nabla c_e = D_e\nabla^2 c_e - kc_p c_e \qquad (4.6)$$

where c_p is the concentration of positive ions, which may be taken to be the concentration of hydrated protons after the initial yield positive ion species have reacted with H_2O. For the case of spherical geometry Eq. (4.6) becomes

$$\frac{\partial c_e}{\partial t} + \frac{\mu \partial \Phi}{\partial r}\frac{\partial c_e}{\partial r} = \frac{D_e}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c_e}{\partial r}\right) - kc_p c_e \tag{4.7}$$

where the electrostatic potential, $\Phi(r)$, is given by

$$\Phi(r) = \frac{4\pi}{r}\int_0^r \left(\frac{e}{m}\right)(c_p - c_e)r'^2 dr' \tag{4.8}$$

The problem of "ambipolar" diffusion with recombination expressed by Eq. (4.6) is an interesting and varied one, to which much attention has been given recently (Christophorou, 1981). A full treatment of this problem will not be attempted here. In its place, one extreme limit of the two which bracket the exact solution will be taken as a working approximation, so that we may get on with things. However, this would be an interesting future direction in which to take this work.

These two extreme limits consist of setting μ equal to 0, on the one hand, and ∞, on the other. In the first case, the electron is not influenced by the field, and only diffuses. In the second case, the influence of the field is overwhelming, and diffusion is bypassed by instantaneous global recombination. The latter course is chosen here. We therefore set f=1 in Eqs. (4.3a) and (4.3g), and invalidate Eq. (4.3e).

The best approximation to the true time course of the concentration of the thermal electron that can be had under these circumstances would

probably be to simply renormalize the initial yield by the factor $1/N(E_o)$, and allow these electrons to simply diffuse.

For this purpose we then need the diffusion coefficient of the thermalized electron through H_2O. Rio (Ph. D. thesis, 1983) observed that it may be estimated from the elastic cross section, extrapolating low energy cross section data of Seng (1975) below .35 eV. Specifically, the mean free path between collisions, $\langle \ell \rangle$, is given by $\langle \ell \rangle = 1/\sigma_{el} n$. The diffusion coefficient is given exactly by $D_e = \langle v^2/3\nu_c \rangle = \langle v\ell/3 \rangle$ (Brown, 1958) where ν_c is the collision frequency, following from its definition as the proportionality constant between the total particle flux and the concentration gradient. The ensemble average can be approximated by neglecting correlation in one of two ways (Reif, 1965):

$$D_e \approx \langle v \rangle \langle \ell \rangle / 3 = (1/3)(8k_B T/\pi m_e)^{1/2}(1/\sigma_{e\ell} n) \qquad (4.9.1)$$

(dimensional estimate)

$$D_e \approx \langle v^2 \rangle \langle \ell \rangle / 3 \langle v \rangle = (1/3)(3k_B T/m_e)(1/\sigma_{el} n)/(8k_B T/\pi m_e)^{1/2} \qquad (4.9.2)$$

(random walk estimate)

These two estimates differ by less than the uncertainty in the extrapolated estimate of σ_{el}. A temperature and density dependent value for D_e follows.

Knowing D_e, we obtain μ via the Einstein relation,

$$D_e = (m/e)\langle v^2/3 \rangle \mu \qquad (4.10)$$

(Allis, 1956; Brown, 1958). It follows then that $\mu/e = D_e/kT$. The general problem of charge separation posed by Eq. (4.7) can now be addressed quantitatively. This problem is left for future work.

Ion Reaction Time Scales

We here attempt to undertake a quantitative treatment of the time scales of the ion reactions and their dependence on medium density and injection rate. Alternatively, we could simply run a kinetic code, such as Rio's, from which Fig. 4.1 was obtained, for a few selected values of medium density and injection rate, and find out this way without any effort--for either the initial pulse or the continuous pulse case. We choose to go the first route out of interest, since the latter one is always available to us, if we need it.

In order to simplify things, we may first of all ignore the primary species OH^+ and H^+ which are produced at about one-tenth the level of H_2O^+. We may therefore ignore reactions b-d. Now, only considering reactions a, e, f, and i, g and h, we may further approximate by combining the various hydrated proton species into one average species. We are left then with reaction a with rate constant unchanged, and an average of reactions i, g and h to which we assign an average rate constant. At lower medium densities, this rate should be shifted down toward the the singly hydrated case (the hydronium ion). At higher medium densities this rate should be shifted up toward the triply hydrated proton.

The proton transfer reaction (a) can be treated as a single body decay because of the constant background of H_2O. The time constant is

found via Eq. 3.6 in the case of initial pulse or Eq. 3.3 in the case of continuous pulse. For the system of Fig. 3.1 (initial pulse) this turns out to be about 10^{-8} sec, which agrees with the figure. (Although not shown, $C_{H_2O} = 10^{-7}$ mole/cc, as can be seen by noting the time course of H_3O^+ and the rate constant for reaction a.)

The reaction time of the electron-proton recombination is found either from Eq. (3.9) in the initial pulse case or from Eq. (3.22) in the continuous pulse case. Equation (3.9) (or its asymptotic case, Eq. (3.6)) does not spell out reaction time. We may do that here, using the e-folding interval as a definition. One obtains

$$\tau_c = \begin{cases} 1/k(c_{10} - c_{20}) & c_{10} \gtrsim 2c_{20} \\ 1/kc_{20} & c_{20} < c_{10} \lesssim 2c_{20} \end{cases} \tag{4.11}$$

For the system of Fig. 4.1 the average rate implies an e-folding time of 6×10^{-8} sec. This is somewhat low. Using the rate for H_3O^+ instead, considering the low density, one obtains 1.3×10^{-7} instead, which is in better agreement.

The above analysis applies to the case in which the reaction time of recombination is later than the reaction time of proton transfer. In this case the reaction time of recombination, the last step, defines a close-out time. In the opposite case the proton transfer reaction is the 'rate limiting step', and defines both onset and close out.

It is convenient to leave this question of the time scales of the ion reactions momentarily in order to go on to a discussion of the

neutral reactions in the next chapter. However, we will return to it at the end of that chapter and complete our discussion of it there.

CHAPTER V
KINETICS OF FULL NEUTRAL REACTION SET

Introduction

The radiological context dictates four degrees of freedom: medium density, injection rate, incident energy and temperature. Room temperature is the most natural choice, especially for the liquid state. In this connection it is important that we make it clear that calculations for liquid density based on spatial yields computed from gaseous phase cross sections and on a gas phase reaction set are only to be considered as extrapolations.

Taking as our point of comparison the spatial yields at r=0 as we had done in Chapter III, two of these degrees of freedom, namely incident energy and injection rate, as a result of the near constancy of g-values for $E_o \gtrsim 100$ eV, combine effectively into one degree of freedom for this corresponding kinetic system--the "strength", or scaling, of the source terms of the assorted species.

If it is a true result that the range of the high spectral plume relaxes as E_o increases, then this fact, along with the clear decrease in the high spectral plume g-value with increasing E_o, can be taken to imply essentially single range, or single exponential, spatial profiles of the yields at higher E_o, say, $E_o \gtrsim 1$ keV. The general picture of spatial profiles of the yields which emerges is then one based only on the total g-value.

For the post-recombination yields, we obtain, from Fig. 2.20, the following relative values of the total g-values:

$$g_H \approx 1.1\ g_{OH},\ g_O \approx 1.3\ g_{H_2} \text{ and } g_H \approx 10\ g_{H_2}.$$

The temperature of 400 K is somewhat arbitrarily chosen to work at. For the liquid density case both 400 K and 300 K are calculated at. Because of the energetics of the reactions in this temperature region, this does not lead to a significant difference in the character of results. That this should be so can be already appreciated from considering Table 4.2 where reaction rates at 300 K as well as 400 K are presented (the general temperature dependences are given in Westbrook, 1981). This can be seen for the third body reactions as well as for the two body reactions.

This reaction set, intended to apply to combustion, is more extensive than we really need for the radiological problem in the vicinity of room temperature. Most of the reactions can be taken as one way in this temperature domain. It is easy to see that this is so for all the third body reactions. That it is so for most of the two body reactions can be seen from Table 5.1 where the ratio of forward rate coefficient to backward rate coefficient or the reverse is given--(the ratio of the larger to the smaller is given). Reaction 2 has the most equal energetic balance. The reactions for which the order of magnitude of the ratio is below 10 may be driven in the reverse direction if the concentrations are just right. This however is the exception. Those for which the order of magnitude is higher yet can be taken as effectively one way reactions. A minimal reaction set which is a subset

TABLE 5.1
Ratios Between Forward and Backward Rate Coefficients
for the Two-Way Reactions

(Ratios are of the larger rate coefficient to the smaller.)

Reaction	Ratio at 300 K	at 400 K
1	4.3(10)	5.3(7)
2	12.0	5.3
3	3.5(11)	2.5(8)
4	2.5(10)	4.4(7)
5	1.3(22)	3.0(16)
8	2.5(40)	1.9(30)
9	1.4(29)	1.6(22)
10	1.8(41)	7.3(30)
11	9.6(51)	5.2(38)
12	5.5(29)	1.4(22)
14	1.8(11)	3.5(8)

of this one can be identified. Rather than bother with this at this point, we will let the kinetic calculations tell us which ones are contributing, since little extra expense is involved in the numerical calculation from more reactions, this coming primarily from number of species.

It should be noted that the favored one-way reactions are all either two body or effectively two body (third body is primarily background H_2O). The two effectively one body decay reactions (3f and 4f) are energetically unfavored.

Principal Pathways and Reaction Times

Setting all yields (i. e. source terms)--for H, OH, H_2 and O--to be of the form, $y_i = A_i e^{-\beta dr} = (\beta_i^3 d^3 I Z_i/8\pi)e^{-\beta_i dr}$, where I is the injection rate, since we want to calculate pure kinetics for the yields obtaining at r=0, we turn our attention on A_i rather than Z_i, the spatially integrated yield. We therefore define a quantity, $S = Id^3$ which we may call the source strength.

We are interested in the variation in the kinetic time courses with medium density, d, and source strength, S. We define dimensionless density, injection rate and source strength in terms of convenient reference values: $h = d/d_o$, $i = I/I_o$ and $g = S/S_o$ where $S_o = I_o d_o^3$ where $I_o = 10^{12}$ #/sec and $d_o = 10^{-8}$ gm/cc = 6.02×10^{15} #/cc.

We now investigate the g-h grid. The grid points (g,h) calculated for are labelled in Fig. 5.1. The kinetic time courses for those labelled by an alphabetic character other than an o are presented in Figs. 5.2a-i, Fig. 5.3j-k, Fig. 5.4ℓ and Fig. 5.5m. These are for post-

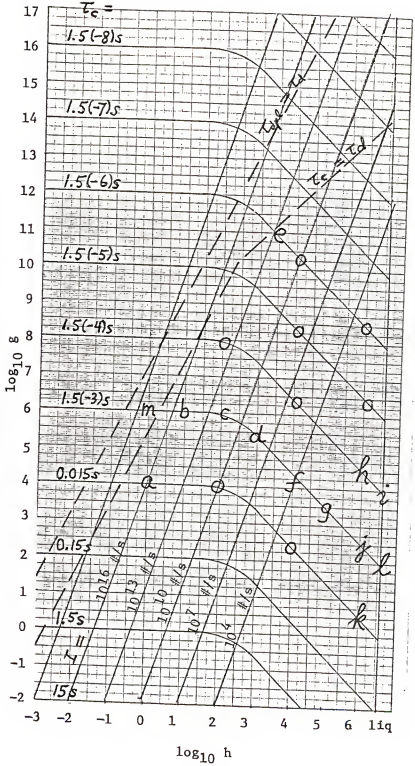


Figure 5.1. Medium density-source strength grid. Overlaid with isocontours of (1) injection rate for equivalent yield at r = 0, (2) kinetic onset time, (3) borderline of fast/slow chemistry, and (4) borderline of depletion regime for diffusion only. Points at which kinetic runs were made are labelled.

Figure 5.2. Kinetic time course of post-recombination neutral system for T = 400 K, E_o = 1 keV, yield rates obtaining at r = 0, for

(a) $g = 10^4$, $h = 1$ (τ_c = .015 sec),
(b) $g = 10^6$, $h = 10$ (τ_c = .0015 sec),
(c) $g = 10^6$, $h = 100$ (τ_c = .0015 sec),
(d) $g = 1.4 \times 10^5$, $h = 10^3$ (τ_c = .0015 sec),
(e) $g = 1.0 \times 10^4$, $h = 3067$ ($\tau_c = 1.3 \times 10^{-6}$ sec),
(f) $g = 1.4 \times 10^3$, $h = 10^5$ (τ_c = .0015 sec),
(g) $g = 1.4 \times 10^4$, $h = 10^6$ (τ_c = .0015 sec),
(h) $g = 1.4 \times 10^4$, $h = 10^6$ (τ_c = .00015 sec),
(i) $g = 2.5 \times 10^3$, $h = 5.57 \times 10^6$ (τ_c = .00015 sec).

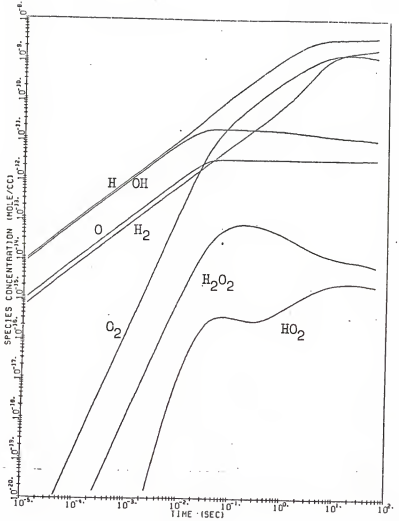


Figure 5.2 (a)

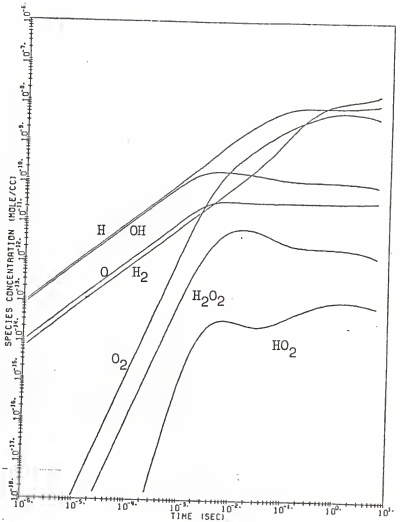


Figure 5.2 (b)

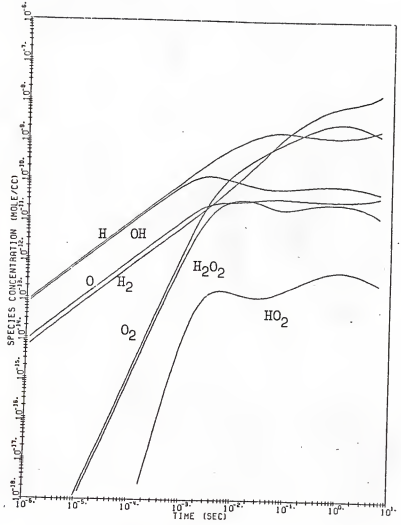


Figure 5.2 (c)

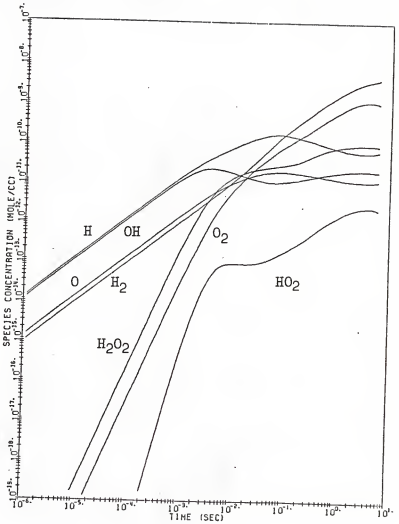


Figure 5.2 (d)

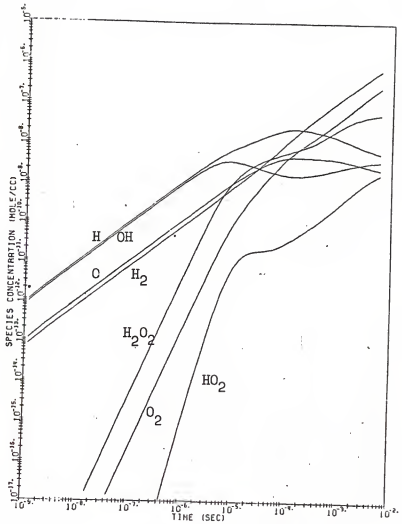


Figure 5.2 (e)

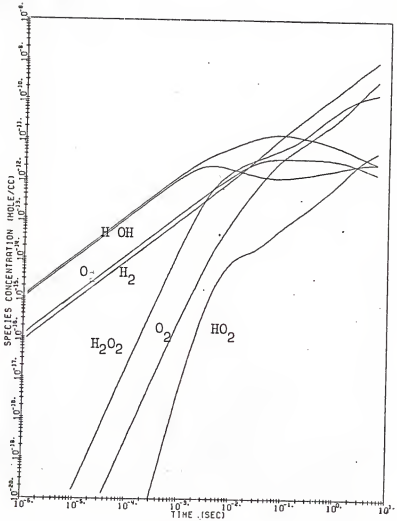


Figure 5.2 (f)

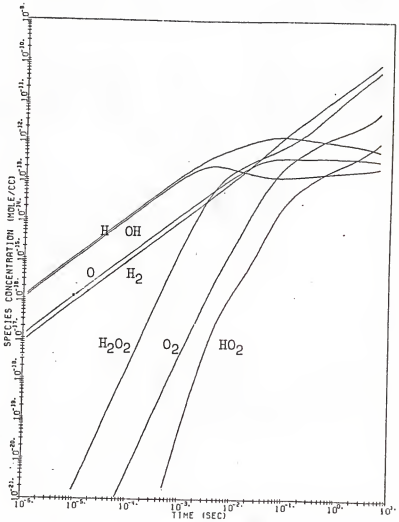


Figure 5.2 (g)

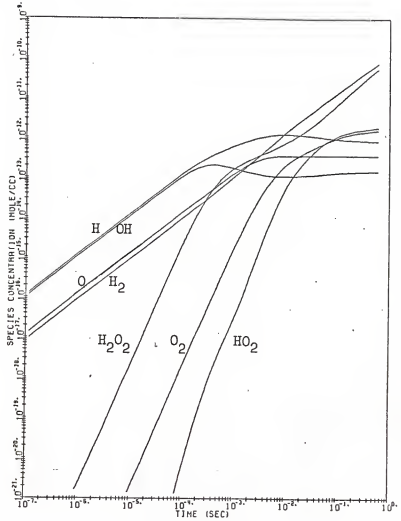


Figure 5.2 (h)

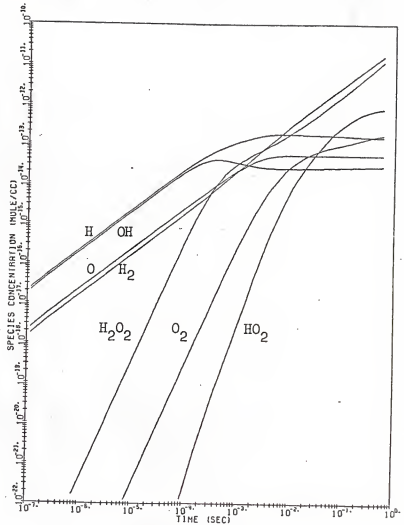


Figure 5.2 (i)

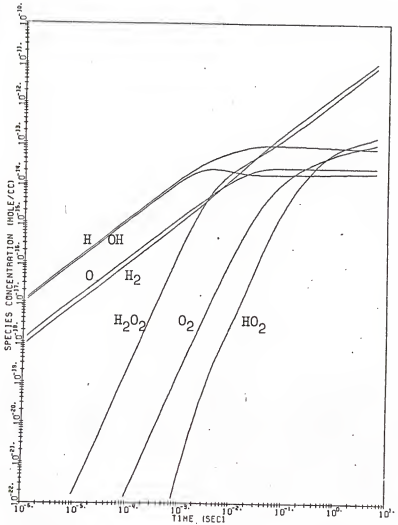


Figure 5.3. Kinetic time courses below the minimum g for convergence of pattern: (j) g = 140, h = 10^6 (τ_c = .0015 sec).

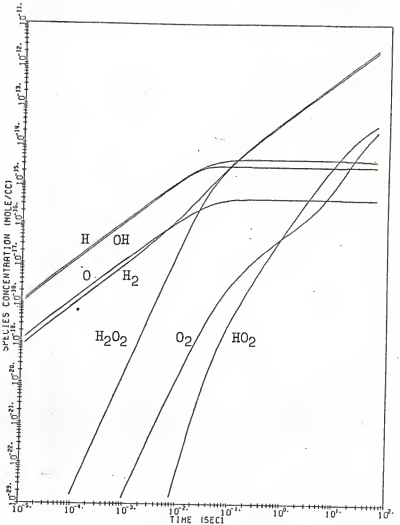


Figure 5.3. Kinetic time courses below the minimum g for convergence of pattern: (k) g = 1.4, h = 10^6 (τ_c = .015 sec).

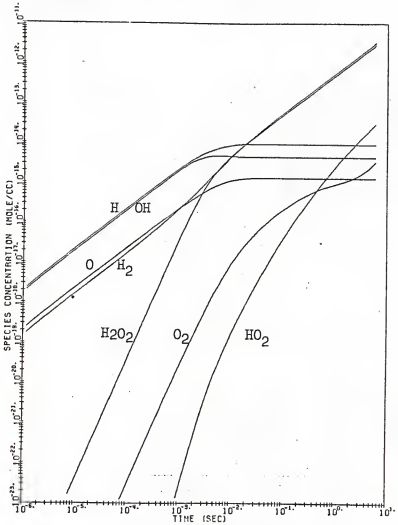


Figure 5.4. Kinetic time course below the minimum g for convergence of pattern:
(ℓ) $g = 250$, $h = 5.57 \times 10^6$
($\tau_c = .0015$ sec).

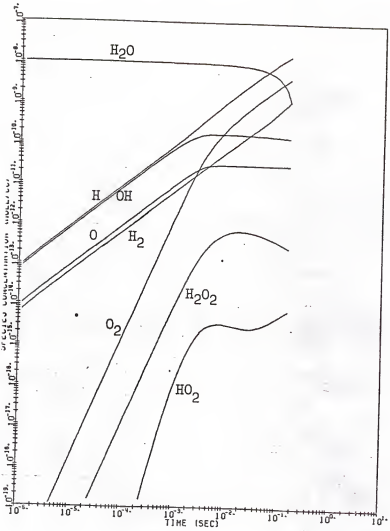


Figure 5.5. Kinetic time course illustrating depletion: (m) $g = 10^6$, $h = 1$ ($\tau_c = .0015$ sec).

recombination spatial yields at T = 400 K and E_o = 1 keV. Fig. 5.6 presents the same system as in Fig. 5.2i (liquid density) except with the difference that it is at 300 K. Systems (a)-(i) with the exception of (e) all have τ_c = .015 sec, .0015 sec or .00015 sec. The choice of g in system (e) is made to agree with the diffusion kinetic system of H + OH in Chapter III and with the second injection rate for the second density considered in Chapter VI. System m illustrates depletion. Choices (j)-(k) and (ℓ) illustrate a significant effect which we did not investigate further. This is the following. In all other cases we observed no variation of pattern of the kinetic time courses with g—only a rescaling of concentration and time scale. However at these low source strengths, we observe the pattern begin to change. This would be an interesting avenue of further study.

In the g-h grid in Fig. 5.1 isocontours of i are plotted from the equation, $g = hi^3$. Thus, noting maximum and minimum physically meaningful values of i, we limit the region of the g-h grid which we are interested in. The mathematical properties of grid points with respect to the associated kinetic systems are, however, independent of these physical considerations. The meaning of unchanging pattern with respect to g above a minimum value can be clarified. This means that only the vertical and time axes need by rescaled.

The evolution of pattern seen in Figs. 5.2a-i is now discussed. We first look at the early time regime. Here chemistry is still only feedforward to the product species, and the reactions which produce them are noted: 1b for O_2, 13b for H_2O_2, and primarily 7f for HO_2. We are more interested in the first two. Since reaction 13b is third body, the

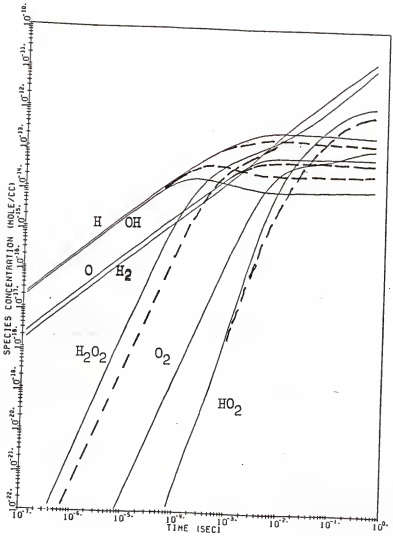


Figure 5.6. Kinetic time course for same yield strength and density (liquid) as in system (i) but at T = 300 K (system (n)). Kinetic time course for system (i) is overlaid (dashed curve).

production rate of H_2O_2 increases with increasing h. H_2O_2 production, below that of O_2 at low densities, is considerably above it at the higher densities.

It is noteworthy that H is fairly unreactive at low densities. The two body reactions it is involved in are not very fast. At higher density, three body (radical recombination) reactions are favored, and H is more reactive in this density regime.

We now home in on three representative cases: system (a), the low density gas; system (e), the 1 atm gas; and system (i), the liquid density case, essentially the extremes and about the midpoint. At each of these densities, we plot the net production rate time courses (including source term). According to the kinetic equations, the net production rate should equal the time derivative of the species concentration. This will be checked. These plots are given in Fig. 5.7 for system (a), Fig. 5.9 for system (e), and Fig. 5.10 for system (i).

In order to identify the dominant reactions, also known as the principal pathways, we have also plotted time courses of individual reaction rates (i. e. the net two body or the associated net effective two body reaction rate). These are given in Figs 5.8, 5.11 and 5.12 for systems (a), (e), and (i), respectively.

Finally, these reaction rates are multiplied by the appropriate signed stoichiometric factors to give production rates of species per reaction. Time courses of these quantities are plotted in Figs. 5.13, 5.14 and 5.15 respectively for systems (a), (e), and (i). The assignment of subfigures is the same in all of these, namely: (a) H, (b) OH, (c) H_2, (d) O, (e) HO_2, (f) O_2, (g) H_2O_2 and (h) H_2O.

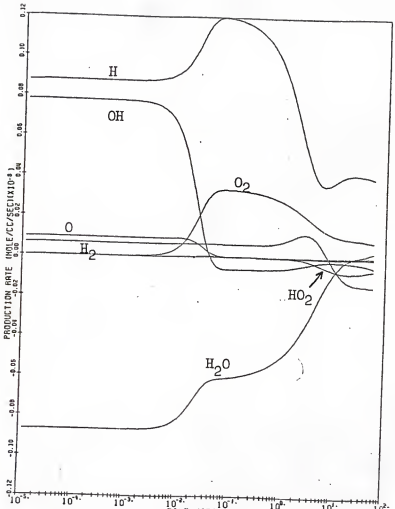


Figure 5.7. Time course of net production rates for kinetic system (a).

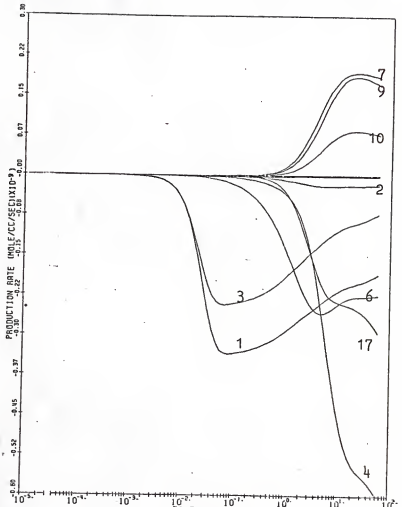


Figure 5.8. Time course of reaction rates for kinetic system (a).

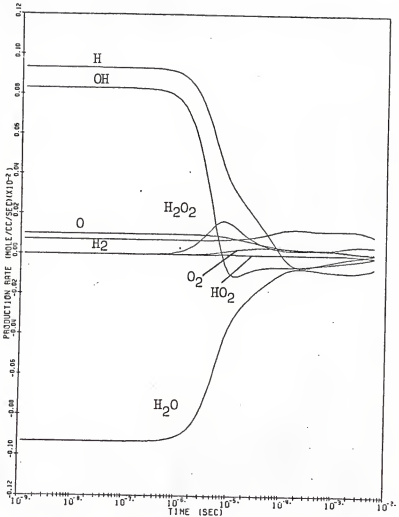


Figure 5.9. Time course of net production rates for kinetic system (e).

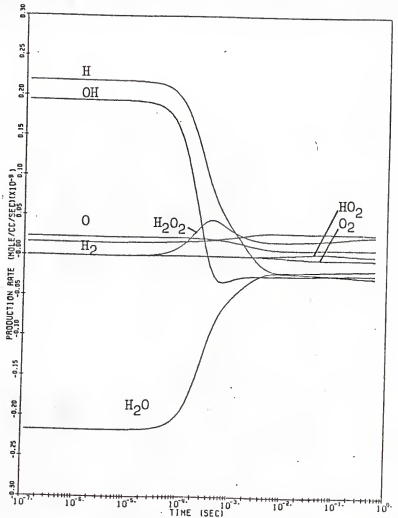
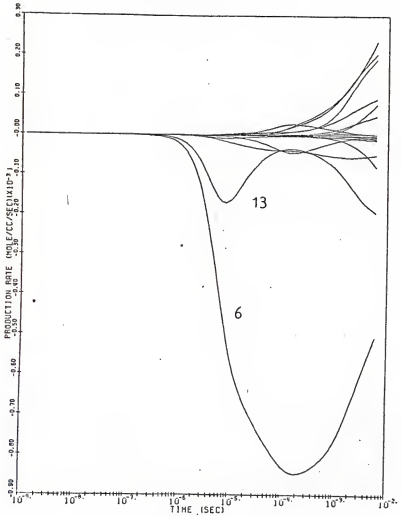


Figure 5.10. Time course of net production rates for kinetic system (i).



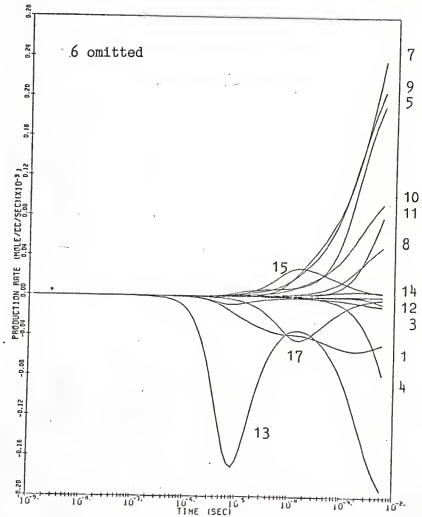
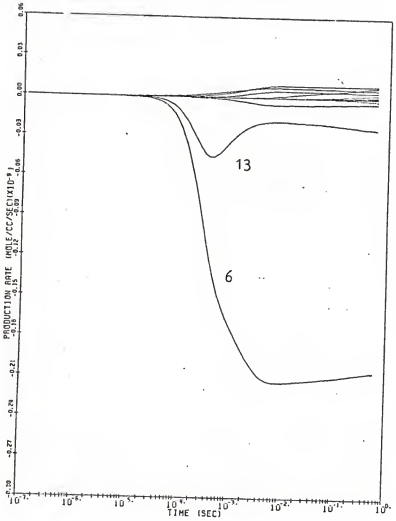


Figure 5.11. Time course of reaction rates for kinetic system (e).



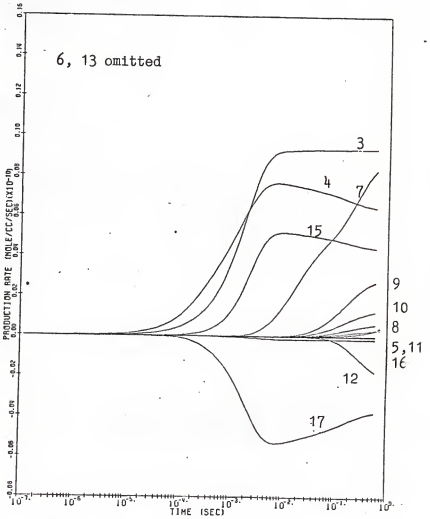


Figure 5.12. Time course of reaction rates for kinetic system (i).

Figure 5.13. Time courses of production rates of (a) H, (b) OH, (c) H_2, (d) O, (e) HO_2, (f) O_2, (g) H_2O_2, and (h) H_2O for kinetic system (a) from each reaction.

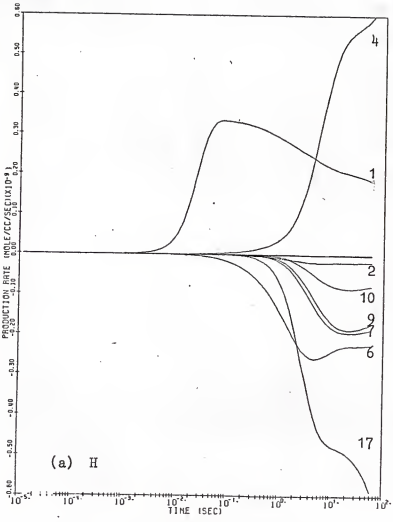


Figure 5.13 (a)

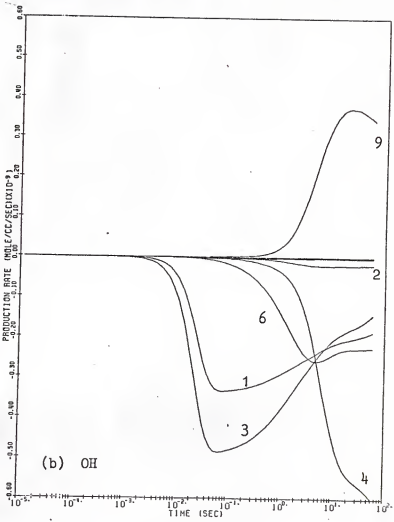


Figure 5.13 (b)

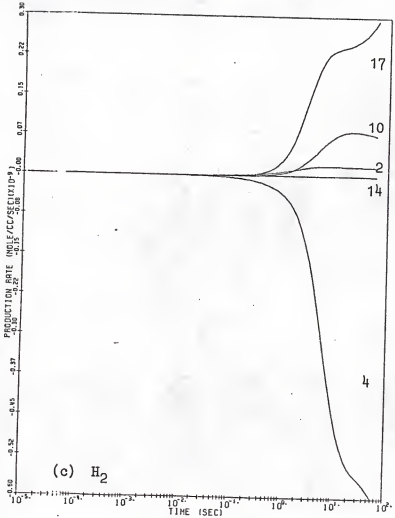


Figure 5.13 (c)

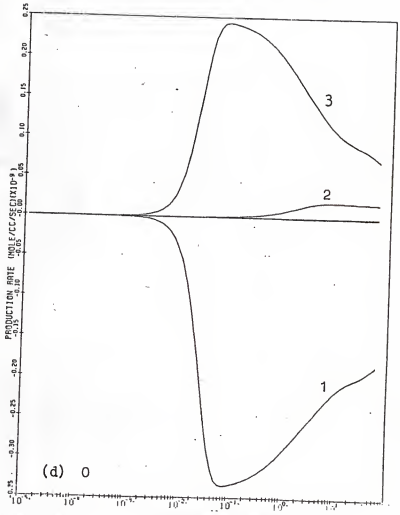


Figure 5.13 (d)

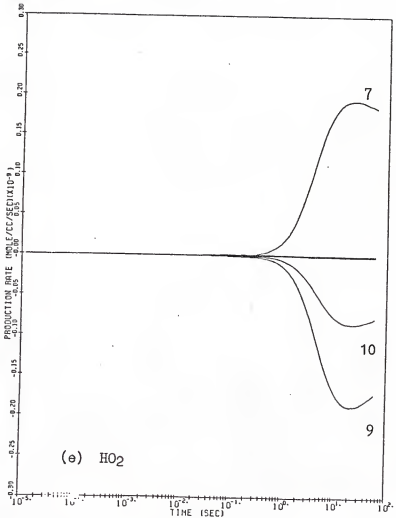


Figure 5.13 (e)

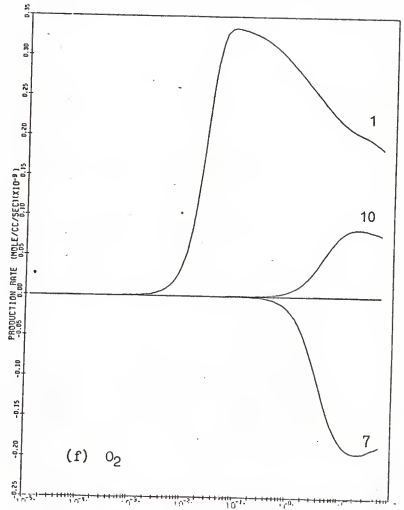


Figure 5.13 (f)

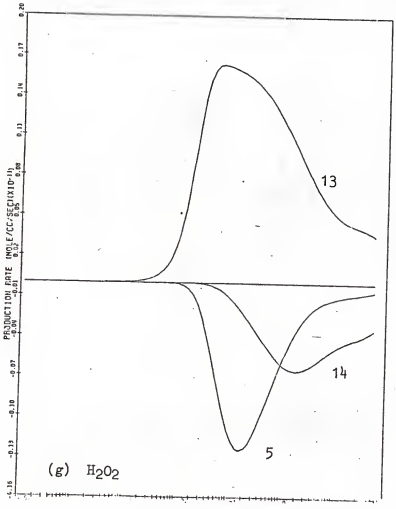


Figure 5.13 (g)

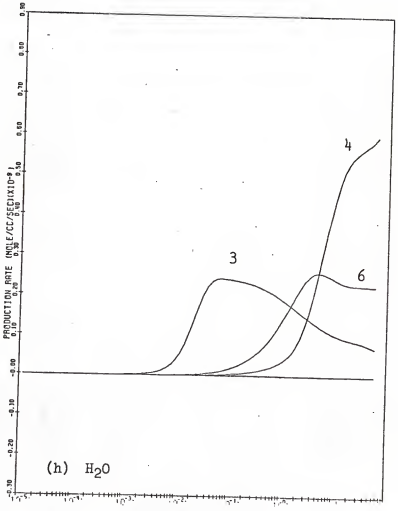


Figure 5.13 (h)

Figure 5.14. Time courses of production rates of (a) H, (b) OH, (c) H_2, (d) O, (e) HO_2, (f) O_2, (g) H_2O_2, and (h) for kinetic system (e) from each reaction.

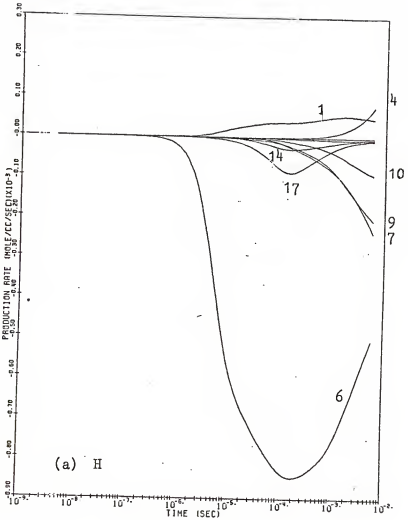


Figure 5.14 (a)

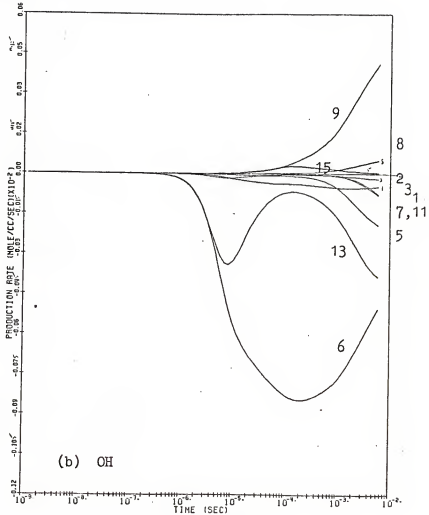


Figure 5.14 (b)

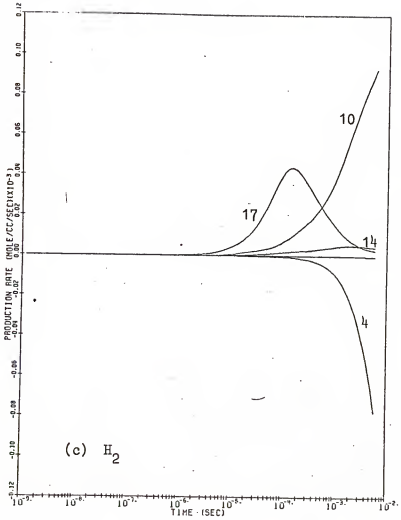


Figure 5.14 (c)

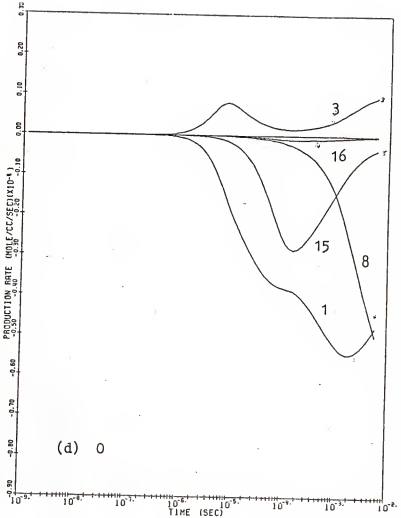
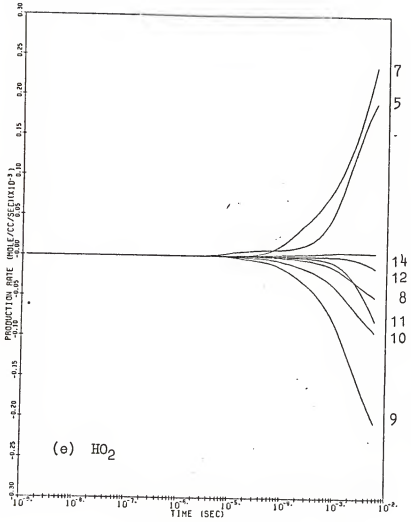


Figure 5.14 (d)



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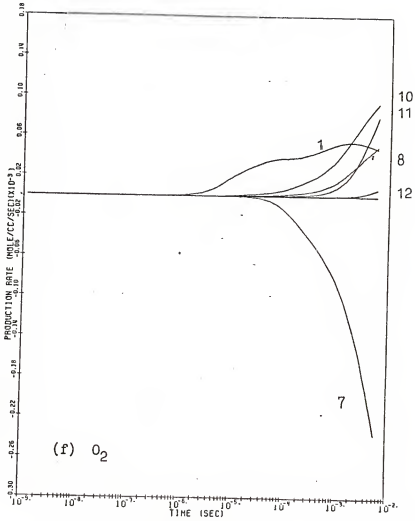

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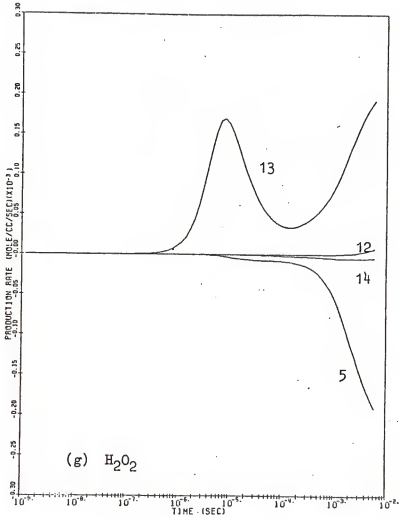


Figure 5.14 (g)

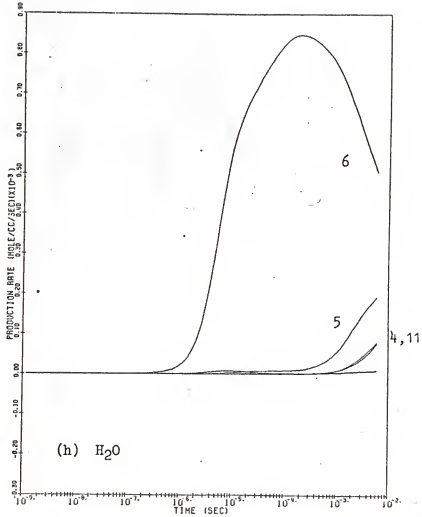


Figure 5.14 (h)

Figure 5.15. Time courses of production rates of (a) H, (b) OH, (c) H_2, (d) O, (e) HO_2, (f) O_2, (g) H_2O_2, and (h) H_2O for kinetic system (i) from each reaction.

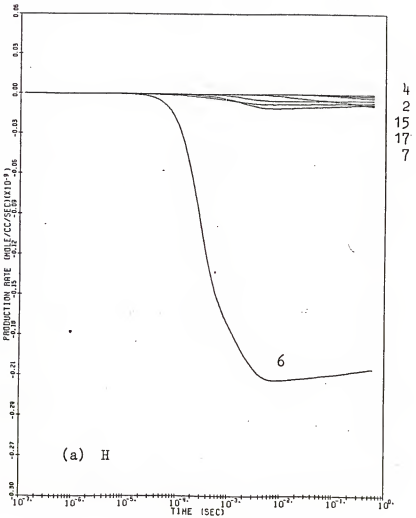
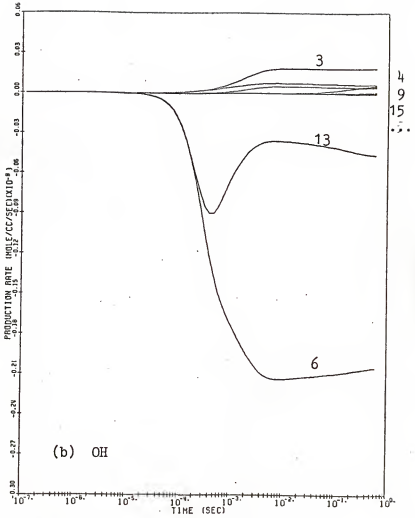


Figure 5.15 (a)



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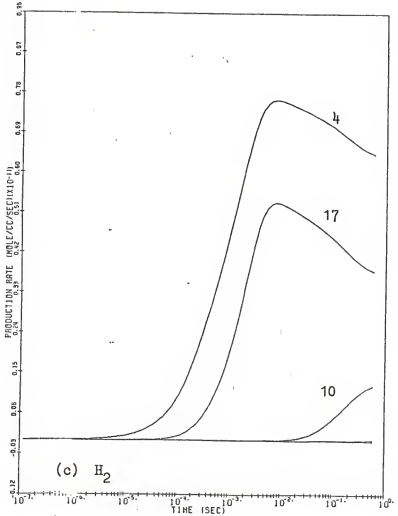

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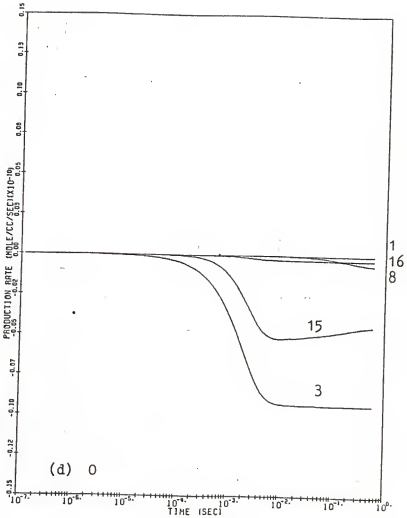

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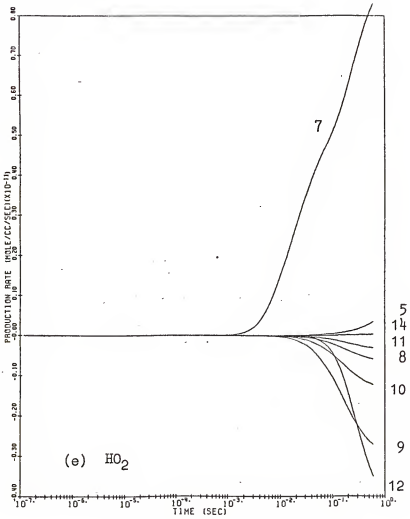

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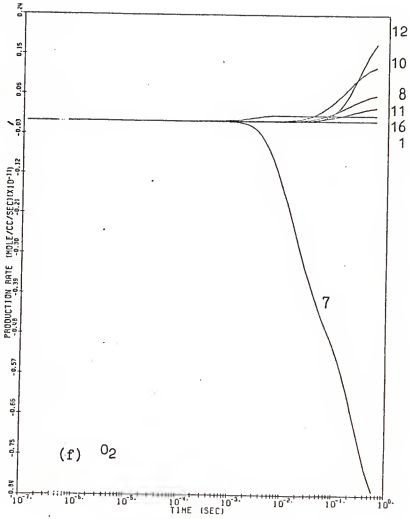


Figure 5.15 (f)

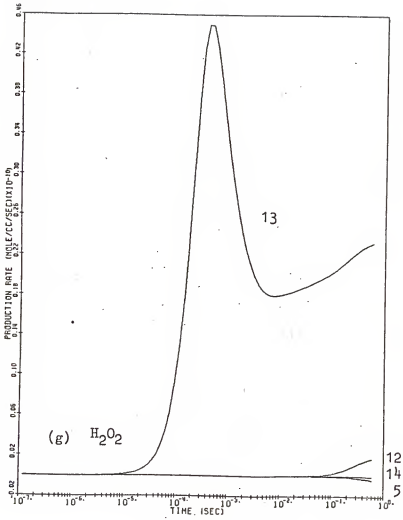


Figure 5.15 (g)

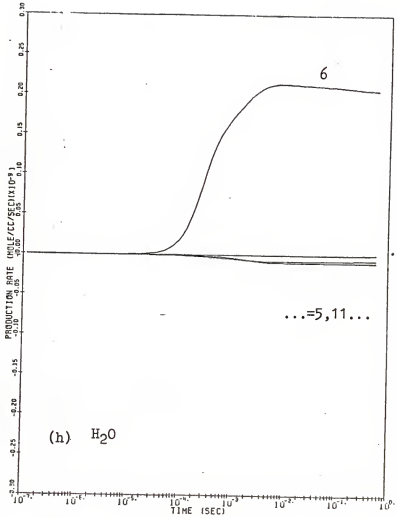


Figure 5.15 (h)

From this series of time courses we can precisely identify the principal pathways overall and in the production-destruction of each species. Let us now describe the more significant features. We may start with the evolution of reaction 6, H + OH recombination, and its weaker companion, reaction 13, OH + OH recombination. In system (a), reaction 13 is barely noticeable, while 6 is of average importance among the principal pathways at the later stage (following the second reaction time in this system). In systems (e) and (i) they are both the strongest two reactions--in system (i) for all time seen, in system (e) until later time when a second group of reactions start up (similar to the situation in system (a)). In system (a), two reactions which are relatively weak in (e) and (i) pre-stage the show by two orders of magnitude in time. These are, namely, reactions 1 and 3.

We may now calculate reaction time. First we look at low density. The reactions 1 and 3 form a feedback loop on OH. The rate coefficient of reaction 3 is lower by a factor of 10 than that of reaction 1. However the ratio of source terms $y_{OH}/y_O = 8$ mostly makes up for it. As a result OH scavenges itself in the net balance about as fast as it scavenges the less plentiful O, and OH is seen to fall off in sync with O, and then continues after the source term supply of O has already been neutralized. The reaction time is given in Eq. (3.22) for this system. We then have

$$\tau_c = 1/\sqrt{k_{1b}(Y_{OH} - Y_O)} \ . \tag{5.1}$$

At higher density, the reaction time is that of reaction 6, and, again following Eq. (3.22), we obtain

$$\tau_c = 1/\sqrt{k_{6b} C_{H_2O} Y_{OH}} \tag{5.2}$$

Substituting in numbers, this comes out to $\tau_c = 1.5/g^{1/2}$ and $\tau_c = 24./(gh)^{1/2}$. These reaction times intersect at h = 256. The h value at which early time H_2O_2 and O_2 production are equal is 140. Contours of constant τ_c are plotted in Fig. 5.1.

In the diffusion kinetic case, it is necessary to know also the diffusion time, τ_d. Recalling from Chapter III that $\tau_d = 1/D\beta^2 d^2 = 1/D_o\beta^2 d_o d = 1/D_o\beta^2 d^2\ h$ $(D = D_o(d_o/d)$, we note that for H, D_o = 6400 cm^2/sec, for OH, D_o = 1830 cm^2/sec (Table 6.1). We may take an average of 4000 cm^2/sec as a fuzzy value in the H-OH recombination region. In the low density region, noting that $D_O \approx D_{OH}$, we set $D_o = D_{OH} \approx D_O$. For E_o = 1 keV, βd_o = .25 cm^{-1}, therefore τ_d = .004/h sec in the first case and .008/h sec in the second. The dependence of the ratio τ_c/τ_d on g and h follows at once. The isocontour $\tau_c/\tau_d = 1$ is plotted in Fig. 5.1.

We may also consider depletion. The time at which $C_{H_2O} = - y_{H_2O}t$, τ_{dpl} is found to be equal to 10^5 h/g (substituting in numbers from the G values given in Chapter II). Comparing against diffusion convergence time in the low density case where diffusion depletion tends to outpace chemistry, this time is significant. However, in the high density region, this time is no longer important because reaction 6 quickly returns much or most of radiolyzed H_2O to its original state. The isocontour $\tau_{dpl}/\tau_d = 1$ is also plotted in Fig. 5.1.

The isocontours plotted in Fig. 5.1, as has been noted, are for E_o = 1 keV and T = 400 K. The complete picture of E_o and T dependence

can be seen from a representative set of these g-h grids, overlaid with isocontours, over the E_o - T grid.

Particle Conservation and the Stiffness Problem

Kinetic systems of equations are famous for the stiffness problem which results if disparate time scales are involved (Dahlquist, Bjorck, 1974; Burden, Faires and Reynolds, 1978). That can easily be seen to be the case here--in systems (a) and (e) a second reaction time manifests itself, while in systems (e) and (i) reaction rates are seen to divide into two groups--a very dominant few and a group of several small ones. In system (e), this group increases in importance at later times.

In order to check the accuracy of our calculations we have done two things. Certainly, this is only a beginning. One was to plot the net production rates, so that we can compare them with the slopes of the concentration time courses. The other is that we calculated the quantity (H atom)/2(O atom) - 1, which measures mass balance (but not necessarily mass conservation). This quantity is graphed in Fig. 5.16 for kinetic systems (a), (b), (c), (f), (h) and (i). Contribution from H_2O species was not taken into account. In the high density cases, since so much of the initial yield of H and OH is recombined, this exaggerated the reading.

In all cases, either because of overproduction of H atoms or underproduction of O atoms (more likely the case because of the levelling off of the reactive radicals OH and O), this ratio increases after reaction time. It peaks at 12-15% for the higher densities, and

Figure 5.16. Time courses of mass conservation in numerical calculation. (H atom)/(O atom) − 2 is the quantity plotted, where H_2O species is not counted. For kinetic systems (a), (b), (c), (f), (h) and (i) in that order.

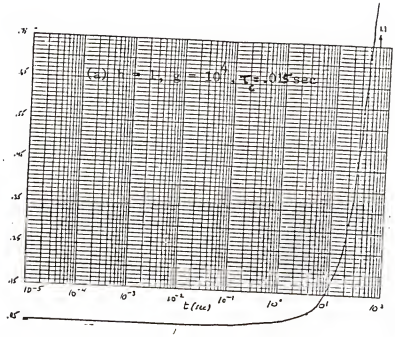


Figure 5.16 (a)

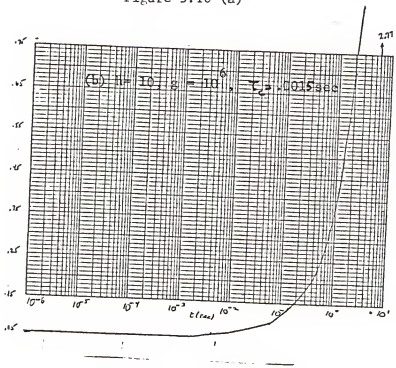
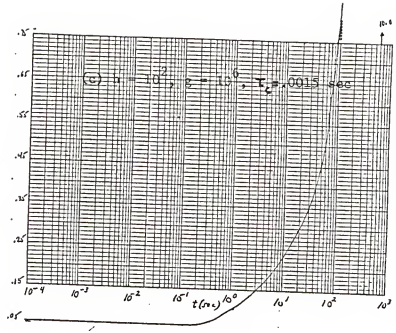


Figure 5.16 (b)



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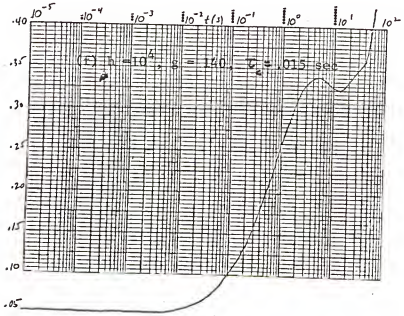


Figure 5.16 (d)

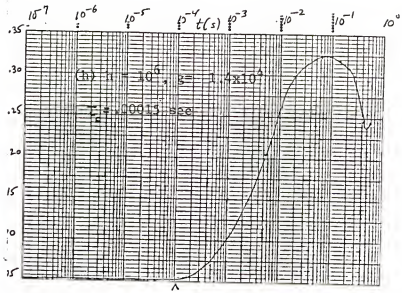


Figure 5.16 (h)

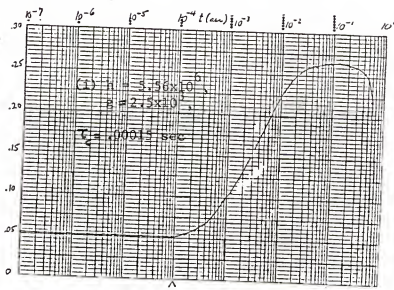


Figure 5.16 (i)

rises like a singularity at the low densities, but at the very later time--after the (first) reaction time it starts its rise slowly.

Comparing the plots of net production rates with the concentration time courses, we observe discrepancies, mostly at later times. These later times are--it should be noted---rather ambitious. Rio (Ph. D. thesis, 1983; see Fig 4.1, this thesis) ran his kinetic code for the full ion-reaction system for initial pulse source term out to about t/τ_c = 200-1000. We are running here for steady source term out to t/τ_c = 40,000.

It is of interest to note here (Rio, private communication, 1983; follow up by author) that the kinetic code he used, which he had adapted from a previous code developed by Walker, Pamidimukkala, Meyreddy and Green, which is based on the Gear method (Hindmarsh, 1974) begins to act up, when calculating for steady source term, around $t \approx \tau_c$. The results it give are strange: the concentrations of the product species start to become jagged in their time courses and even assume negative values intermittently which in their absolute value are nearly continuous with their general trends.

Returning to the plots of net production rates, we consider two examples, the HO_2-O_2 subsystem in system (i) (it is incipient in system (e)) and the time course of HO_2 in the low density case. Looking to Fig. 5.10 in the first example, we see the net production rate of O_2 go negative from initial value of zero (while that for HO_2 does the opposite). This conflicts with the positive definiteness of its concentration time course. From Fig. 5.15e and f it is apparent that

reaction 7 is the source of the problem. We also notice the unlikely way in which reaction rate 7 cuts across the other reaction rates in Fig. 5.12.

Looking at Figs. 5.7 and 5.13e in the second example, we see the net production rate of HO_2 fall from an initial value of zero, conflicting with the positive definiteness of the concentration time course. We see the problem in Fig. 5.13e--the net production rate is the small difference of large quantities. Both of the above examples are examples of stiffness.

The consolations are (1) that the discrepancies occur for the species in lower concentration, and (2) that the overall trends or dominant trends are calculated to an adequate level of accuracy, and (3) the calculation is numerically stable so at least some answer is given. That this is so is a result of the implicit, linearized calculation of the nonlinear kinetic production-destruction terms (see Appendix A), which is known to be numerically stable (Dash and Pergament, 1978; Dahlquist and Bjorck, 1974).

There is perhaps a fourth consolation. Our reason for interest in the kinetics is to base a comparison with diffusion kinetics. The important question then becomes --how does diffusion affect the stiffness problem? Since the effect of diffusion is to slow down the chemistry by placing an upper bound on the growth of the concentration levels of the reactants, it would seem reasonable to conjecture that the effect of diffusion on the stiffness of the kinetic system is one of mitigation. It would be interesting to attack this question rigorously.

Temperature Sensitivity

In order to exhibit the effect of dependence on temperature, the kinetic time course of the same kinetic system as system (i) (liquid density at 400 K) only with temperature changed to 300 K (this system will be denoted as system (n)) has been plotted in Fig. 5.6. The kinetic time course of system (i) is overlaid for the sake of easy comparison. The sensible differences between the two systems are visible from this figure. Overall, taking into account the distortion of log vertical axis, the general trends are unaffected.

Specifically, we note: (1) initial H_2O_2 production increased by a factor of about eight (reflecting the increase in rate constant--see Table 4.2), (2) somewhat earlier reaction time, (3) lower final levels of H, O, and OH, decreased by factors of 2, 0.5, and 2.5, respectively. Initial O_2 and HO_2 production rates are unaffected. Later time O_2 production rate is also unaffected. However, later time HO_2 ambient level is down by factor of 2.

Net production rates are graphed in Fig. 5.17, reaction rates in Fig. 5.18, and reaction-specific production rates in Fig. 5.19, in like manner as the three systems previously detailed. Two distinct energetic effects are noted: (1) most third body radical recombination reactions are speeded up (two are unchanged), and (2) all two body reactions are slowed down in both directions, however with the preferential sense retained, and the general order of magnitude neighborhood of the preferential sense also retained (see Table 5.1).

The die off of two body reactions is most strikingly illustrated by the cases of reactions 3 and 4, which have completely disappeared. The increases in third body reaction rates are far from proportional. This

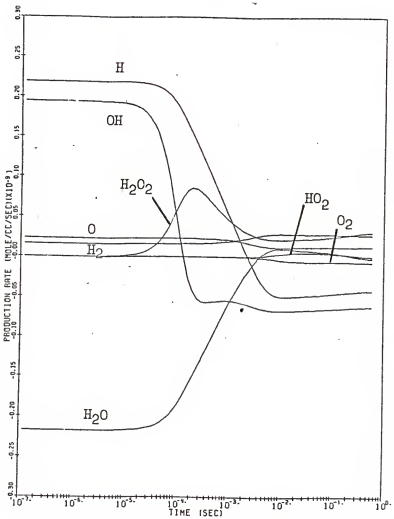
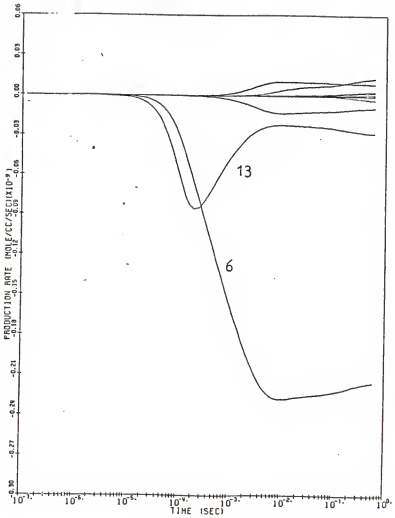


Figure 5.17. Time coure of net production rates for kinetic system (n).



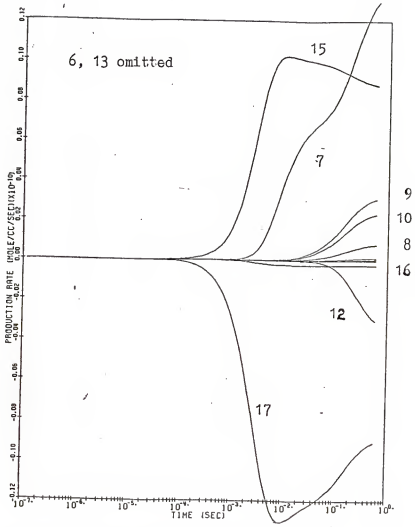


Figure 5.18. Time course of reaction rates for kinetic system (n).

Figure 5.19. Time course of reaction-specific production rates of (a) H, (b) OH, (c) H_2, (d) O, (e) HO_2, (f) O_2 (g) H_2O_2, and (h) H_2O for kinetic system (n).

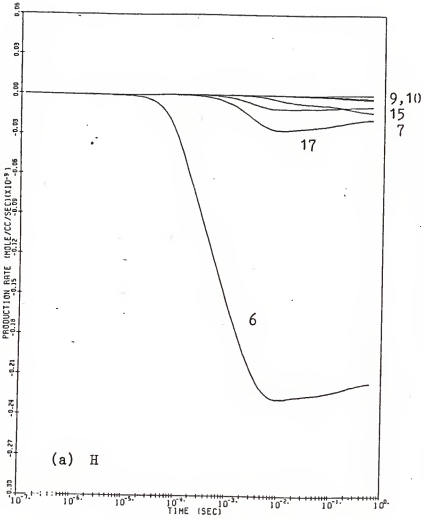


Figure 5.19 (a)

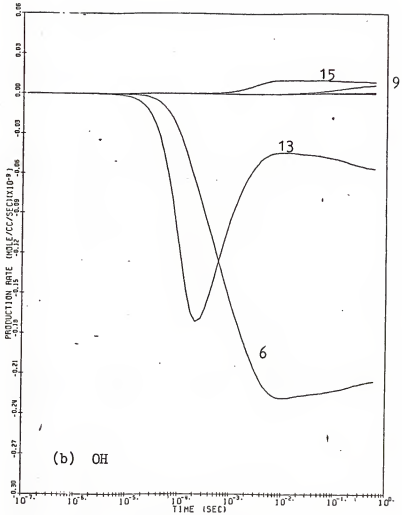


Figure 5.19 (b)

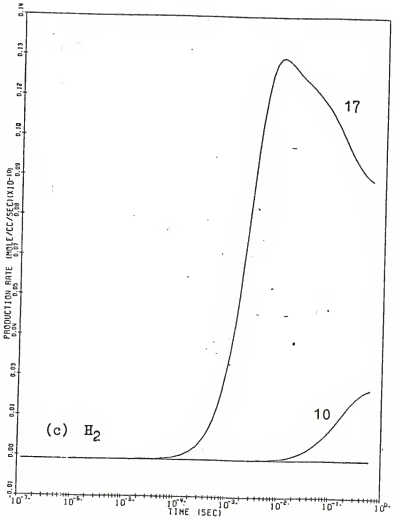


Figure 5.19 (c)

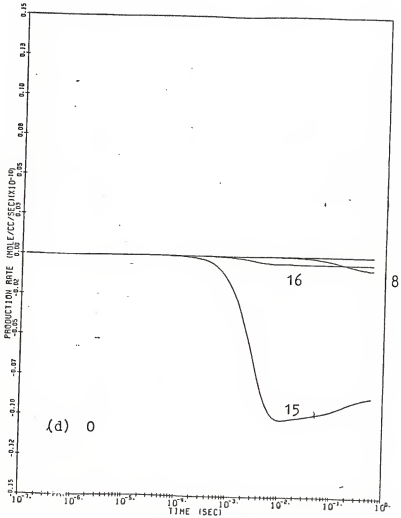
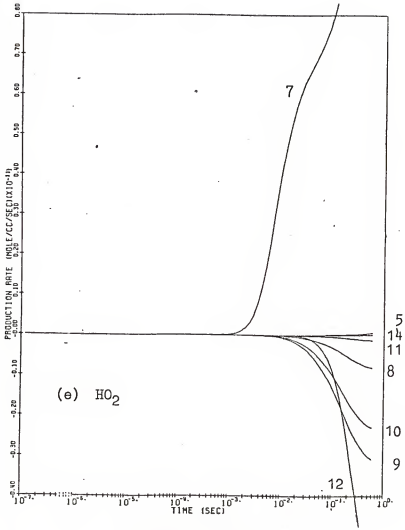


Figure 5.19 (d)



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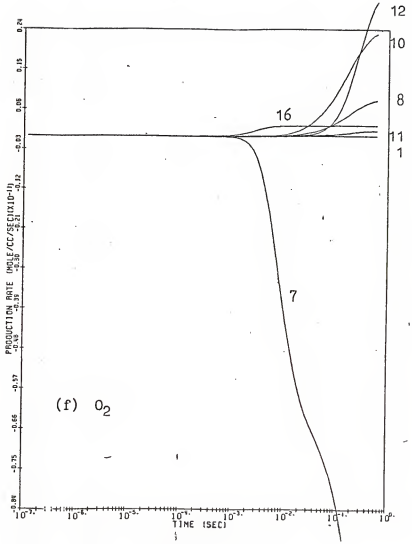

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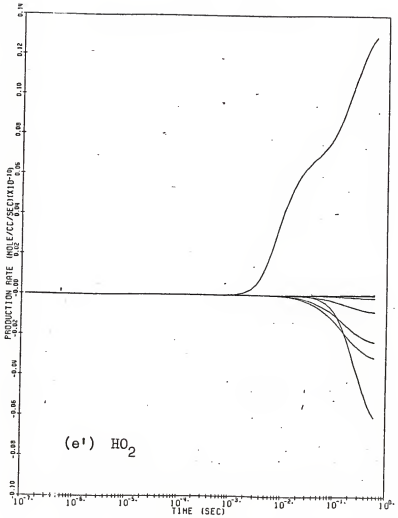

Figure 5.19 (e')

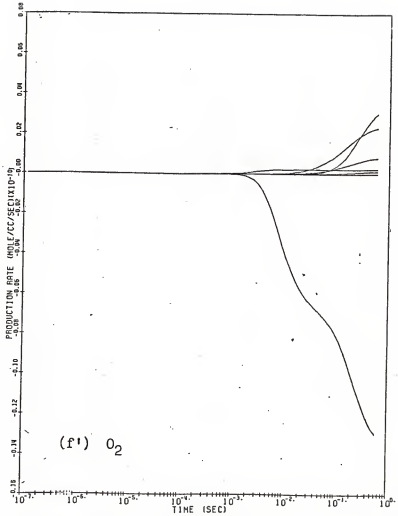

Figure 5.19 (f')

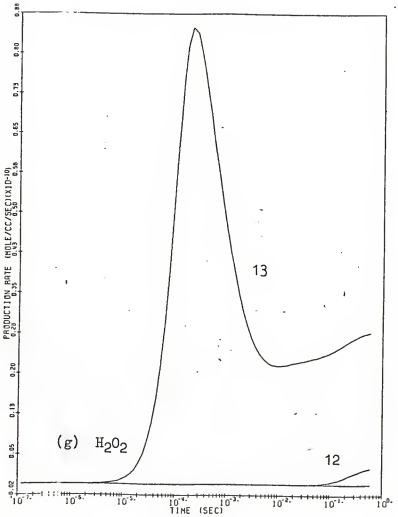

Figure 5.19 (g)

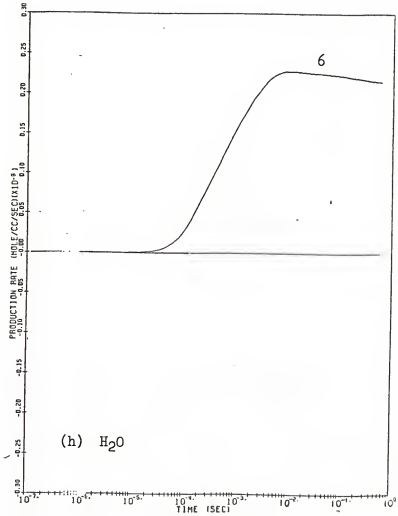

Figure 5.19 (h)

is most notable in the case of H + OH and OH + OH (reactions 6 and 13). The ratio goes from 0.6 at 400 K to 3.0 at 300 K. The effect is significant: reaction time now is keyed to the latter reaction rather than the former, and the transient spurt of H_2O_2 production is doubled in peak height, as a result of which initial OH destruction comes primarily from H_2O_2 production, whereas at 400 K, it comes equally from H_2O_2 and H_2O production. This can be seen by comparing Figs. 5.15 (b) and 5.19 (b).

Separation of Ion and Neutral Time Scales

Now let us pick up where we left off with the ion reaction time scales. We will first compare time scales for incident energy of 1 keV and T = 400 K. We will then also consider T = 300 K. Quantitative results will be expressed in terms of the convenient units of source strength, medium density and injection rate, g, h and i, defined two sections back. By use of the quantity, "source strength," we imply conditions at r=0.

We first note the reaction time for reaction a (proton transfer: $H_2O^+ + H_2O$), given by

$$\tau_{pt} = 8.8 \times 10^{-8}/h. \tag{5.3}$$

Next we note the reaction times for reactions i, g and h (hydrated proton-electron recombination), given by

$$\tau_{e-p} = \begin{cases} .0052/g^{1/2} & (H_3O^+) \\ .0036/g^{1/2} & (H^+(H_2O)_2) \\ .0028/g^{1/2} & (H^+(H_2O)_3) \end{cases} \tag{5.4}$$

We may ask, given a particular density, for what physically possible injection rate (i. e., one which does not cause local depletion the medium, much less give rise to local heating or arcing) does the recombination reaction outpace proton transfer? (This question was asked before in Chapter IV. We are now going to answer it.) To answer this question, we set $\tau_{pt} = \tau_{e-p}$, implementing an average value of τ_{e-p}, which implies

$$g = 1.5 \times 10^9 h^2, \text{ equivalently,}$$
$$i = 1.5 \times 10^9/h. \tag{5.5}$$

Because of the geometric factor, this injection rate decreases with increasing density. For the case of liquid density, Eq. (5.5) implies an injection rate of $2.7\text{x}10^{14}$ #/s or a current of 17 μa. The reaction time is then $1.6\text{x}10^{-14}$ sec for both reactions.

<u>Neutral reaction time</u>. The reaction times of the neutrals at 400 K in terms of g and h are given in section 1. We may repeat them here:

$$\tau_c = \begin{cases} 1.5/g^{1/2}, & h < 256 \\ 24/(gh)^{1/2}, & h > 256,\ f = 1\ . \end{cases} \tag{5.6}$$

It should be noted that the reaction time for $h < 256$ is independent of f, the degree of charge recombination, since H radical is not involved. The reaction time for $h > 256$ does depend on f somewhat at 400 K, but not at 300 K where OH + OH recombination outpaces H + OH recombination. At 400 K, the difference between the H + OH reaction time for f=1 and for f=0 can be detailed. Referring to the graphs of initial and post-recombination g-values at the end of Chapter II, and to Eq. (4.3a), we find that the yield rate for H is increased by a factor of 3 in changing f from 0 to 1. As a result, we find that the reaction time of H + OH is decreased by a factor of $1/\sqrt{2}$ (see Eq. (3.22)). Since OH would move in to take the place of the missing H in the case f=0, it follows, noting the different reaction rate, that the reaction time is delayed only by 20%, not 40%. At 300 K, reaction time for $h > 256$ is given by

$$\tau_c = 11/(gh)^{1/2}. \tag{5.7}$$

For liquid density, this becomes

$$\tau_c = .0047/g^{1/2} . \tag{5.8}$$

Thus, at liquid density the separation of ion and neutral time scales has disappeared. In fact the close-out time of charge recombination exactly dovetails with the onset time of radical recombination, that is, for $i < 270$, equivalently, $I < 17$ μa, or equivalently, $g < 4.6\times10^{22}$. Referring to Fig 5.1, we note that this is already extremely into the

early chemistry region of the g-h grid: the early/late chemistry border stands around $g = 10^{14}$, or equivalently, $i = 6\times10^{-7}$, for the liquid density (to within 20% for T = 300-400 K).

From the above it is clear that at all injection rates in the liquid case adequate time separation of charge recombination and the neutral reactions cannot be assumed. At much higher injection rates, adequate separation in time of proton transfer and charge recombination cannot be assumed, either. This latter point is not so interesting, since such injection rates are not typical. The previous point, however, provides still more motivation to upgrade the code, DIFKIN, to account for local charge recombination--a point that was mentioned in Chapter IV.

In the gaseous case, up to high pressures near liquid density, the separation in time scales between ion and neutral reactions is there. In this case, the motivation to include charge recombination arises only from spatial charge separation.

CHAPTER VI
DIFFUSION KINETICS OF FULL NEUTRAL REACTION SET

Representative Cases

Diffusion kinetics are calculated for the three representative densities chosen in Chapter V, at one of which diffusion kinetics of the single reaction H + OH + M --> H_2O + M was considered in Chapter III. As in effect in Chapter III, we consider three injection rates at each density: for which we have fast, borderline and slow chemistry, specifically $\tau_c = \tau_d/10$, $\tau_c = \tau_d$, and $\tau_c = 10\tau_d$. This is with the exception of the low density at which only two cases are considered: slow: $\tau_c = 1000\tau_d$ and somewhat fast: $\tau_c = \tau_d/2.5$.

The diffusion coefficients have been calculated according to Chapman-Enskog theory (Hirshfelder, Curtiss and Bird, 1953; Monchick and Mason, 1961) utilizing the molecular parameters compiled by Warnantz, Miller and Kee (1983). They are given in Table 6.1.

A schematic of cases (1,h,T), equivalently, (g,h,T) and a guide to figures is given in Table 6.2. These cases are also shown as points on a g-h grid in Fig. 6.2, fitted out with isocontours of τ_c, τ_c/τ_d and τ_{dpl} as in Fig. 5.1.

Before comparing these systems, it is necessary that the first system be mapped into the corresponding system for which $\tau_c = 10\tau_d$. Since we are interested only in the relative values of the concentrations we simply multiply the product species concentrations by the appropriate factors that bring them into the correct relationship with the initial yield species. Those factors are 1400 for O_2 and H_2O_2 and 2×10^6 for HO_2.

TABLE 6.1
Binary Diffusion Coefficients in H_2O
(in units of cm^2/sec)

species	D_1	D_o
H	1.292	6395.
H_2	.8644	4279.
O	.3754	1858.
OH	.3695	1829.
H_2O	.2502	1238.
HO_2	.2339	1158.
H_2O_2	.2327	1152.
O_2	.2305	1141.

D_1 is diff. coef. at $p = p_1 = 1$ atm and $T = T_1 = 300$ K
($n = n_1 = 2.45 \times 10^{19}$ #/cc)

D_o is diff. coef. at $n = 6 \times 10^{15}$ #/cc and $T = 400$ K, i. e.
at $h = 1$ and $T = 400$ K.

$$D = D_1(T/T_1)^{1.67}/(p/p_1)$$

$$= D_1(T/T_1)^{0.67}/(n/n_1) \qquad (p = nk_BT).$$

TABLE 6.2
Schematic of Diffusion Kinetic Systems
and Guide to Figures

h, T & τ_d	slow	border	fast
h=1 T =400 K τ_d =.004 s	t=1 τ_c =1.5 s		t=10 τ_c =.0015 s
	6.2,6.3,6.18		6.4,6.5,6.19
h=3067 T=400 K τ_d =1.3(-6) s	t=.0367 τ_c =1.3(-5) s	t=3.67 τ_c =1.3(-6) s	t=367. τ_c =1.3(-7) s
	6.6,6.7,6.20	6.8,6.9,6.21	6.10,6.11,6.22
h = 3.34(6) T=300 K τ_d=1.2(-9) s	t=1.44(-9) τ_c =1.2(-8) s	t=1.44(-7) τ_c=1.2(-9) s	t=1.44(-5) τ_c =1.2(-10) s
	6.12,6.13,6.23	6.14,6.15,6.24	6.16,6.17,6.25

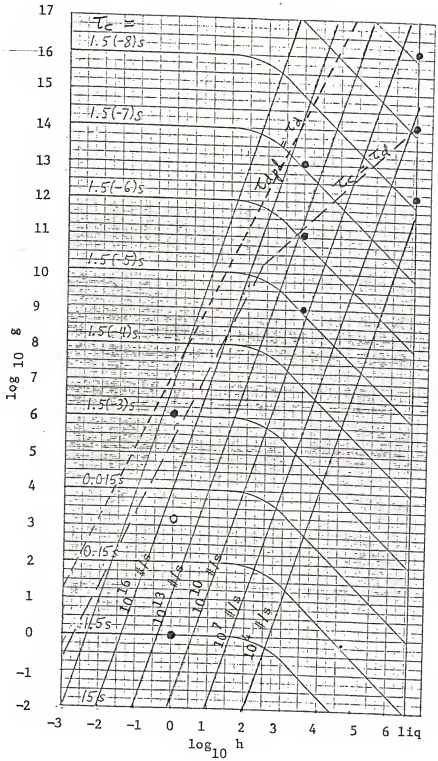

Figure 6.1. Medium density-source strenth grid. Points at which diffusion kinetic runs were made are indicated.

Comparison of Time Courses.

Comparing first of all three time courses for slow chemistry ($\tau_c = 10\tau_d$) we note that in general the majority product species--O_2 or H_2O_2--just crosses the lower range of concentration levels of the initial species (i.e. for H_2 and O) at the last time on the graph, well after the concentrations of all these initial yield species have converged as a result of diffusion.

Looking next at the borderline cases (1 atm and liquid density), we see that for the 1 atm case OH and to a lesser extent H shows some effect of chemistry in their time courses, while both show about equal effect for the liquid density case.

In the low density, somewhat fast chemistry case, it can be seen that OH and O both show a strong effect, and H_2O_2 and HO_2 also by transmission of effect from OH and O (OH is precursor of H_2O_2; OH and O are precursors of O_2 which reacts with H to yield HO_2).

We may next compare the borderline and fast chemistry cases with the corresponding pure kinetic cases (Figs. 5.2a, e and i).

1. In the low density case the difference diffusion makes is that the fast diffusing species, H and H_2, level off.
2. In the 1 atm case and liquid density cases, the fast chemistry case was chosen to be faster than in the low density case ($\tau_c = \tau_d/10$ as opposed to $\tau_c = \tau_d/2.5$). The choice of a lower injection rate in the low density case was not completely arbitrary. Looking to the medium density-source strength grid (Fig. 6.1), one notes that this injection rate is already near the depletion limit. For these fast chemistry cases, the time

courses, as one would expect, continue for a longer time to parallel the corresponding pure kinetic time courses.

Comparison of Radial Profiles.

The slow chemistry profiles are given for the sake of comparison. Otherwise they provide no intrinsically new information. Let us first consider the fast chemistry case at low density. The H profiles are essentially pure diffusion profiles. H is unreactive at this low density, as noted. The profiles of OH and O are almost identical to each other, other than for a scaling factor. This reflects the role of reaction 3. Thus O present at later times becomes primarily more and more O split off from OH, rather than initial yield O. It would be interesting to calculate age distributions.

We next consider the profiles of H_2O_2, HO_2 and O_2, referring to Figs. 5.13 e, f and g for comparison. Let us consider first the profiles of H_2O_2 and O_2. The reactant species which produce them (OH; O and OH) have essentially conformal profiles. They themselves have nearly identical diffusion coefficient. Their profiles differ in shape, that of O_2 reflecting an inert species, which it is, that of H_2O_2 indicating some degree of chemical destruction, reflecting the fact that H_2O_2 is scavenged by OH and H (reactions 5 and 14 — see Fig. 5.13g).

We may compare the borderline and fast chemistry profiles at 1 atm with the corresponding profiles at 1 atm in Chapter III for the isolated reaction, $H + OH + M \longrightarrow H_2O + M$. There are but only slight differences

in the H and OH levels. Referring to Fig. 5.14 a and b, we note that this is already the dominant reaction for both H and OH at this density already.

We next consider the liquid case. Here the borderline case is also not extremely interesting. Going on to consider the fast chemistry case, we observe that the depression of the OH peak in comparison with the H peak is even greater here than in the 1 atm case.

In contradistinction to the low density and 1 atm case, in the liquid density case O is slow to react, and its profiles look essentially like pure diffusion contours. Looking at Fig. 5.19d, we note only one destruction reaction (15), which offsets only one third of the source term for O. As one can see from Fig. 5.18 (reaction rates), not much else is happening in the liquid density case, other than for H + OH and a brief transient in OH + OH recombination. That the radiolysis of liquid water by an electron beam is very slight was observed historically by Lea (1946, 1947).

Comparison of Near Steady State Results

It was noted in Chapter III—in regard to the simple diffusion kinetic system of the single reaction, H + OH, that the most physically realistic or depictive presentation of the results is given by a time sequence of radial profiles of all species together. Each of these plots is a snapshot of the system at a specific time. For the case of a continuous, steady electron beam, this time sequence would depict the approach to steady state. Thus, in this case, the steady state snapshot is of particular interest.

Because it becomes expensive to run the code out to extremely long times, it is necessary to settle on near-steady state results. This is a small detraction. For only-diffusing species, the time course is known, anyway. In the case of fast chemistry the convergence on steady state is abrupt in the core and earlier in the limb than in the only-diffusing case. The treatment in Chapter III is indicative.

Snapshots of near steady state at the last time calculated for in all eight cases are shown in Figs. 6.18-25. In the very slow chemistry case (Fig. 6.18), the full steady state profiles for the only-diffusing species (the 'initial yield' species) are overlaid.

In order to facilitate more meaningful intercomparison between densities, it would have been advantageous to have implemented equal reduced final times (all cases at a given density were taken out to the same final time). Something close to this was done. Noting that $t' = D\beta^2 d^2 t = D_o \beta^2 d_o^2 ht = 250ht$ (using $D_o = 4000\ cm^2/s$), the reduced final times for the three densities, $h = 1$, $h = 3067$, and $h = 5.56 \times 10^6$ (liquid), are 250, 268, and 150, respectively. Since restart diskfiles were recorded to tape for all runs made, the runs at liquid density can be continued to $t' = 250$, should it be desired.

By means of these snapshots of near steady state profiles, it is easier to make qualitative comparisons, for example, regarding level of H_2, H_2O_2 or O_2 production, comparison of those levels with the final ambient levels of the radical species, H, OH, O and HO_2--both with respect to densities and with respect to injection rate at a given density, and so on.

At a quick glance, we note the following significant features. (1) For both the 1 atm cases and the liquid density cases, OH can be seen to fall off more steeply in the borderline case than in the late chemistry case. In the early chemistry case this fall off becomes still more steep. The relative peak level is significantly decreased as well. (2) In the borderline and fast chemistry cases, the stable or relatively stable products and the radicals are generally mixed together in order of magnitude range. No simple formula differentiates them. In the fast chemistry cases (at 1 atm and for liquid density), OH and HO_2 are present at levels significantly lower than for any of the other species. In the case of OH, this reflects its high reactivity. For HO_2, it reflects its low production rate. (3) The peak steady state concentration levels for both the 1 atm fast chemistry case and the liquid density fast chemistry case are both in the same order of magnitude range (10^{-9} - 10^{-7} mole/cc). The reason for this is as follows. Both are 'fast chemistry' cases, i. e., $\tau_c = 0.1\ \tau_d$. Recalling the formulas for τ_c and τ_d, this relation between τ_c and τ_d implies the following relation between g and h: $g/h = 250$. Noting that the final levels are roughly proportional to $g\tau_c$, since levelling off occurs right around or not too long after, it follows that these levels are proportional to $(g/h)^{1/2}$.

Other systematics could be gleaned from these snapshots with more effort. However, many of the more interesting aspects of these diffusion kinetic systems are time dependent in nature, and can only be apprehended in that context. These include (1) the pure kinetic basis for comparison with the full diffusion kinetic case. the analysis in the previous paragraph in terms of fundamental time dependences, namely,

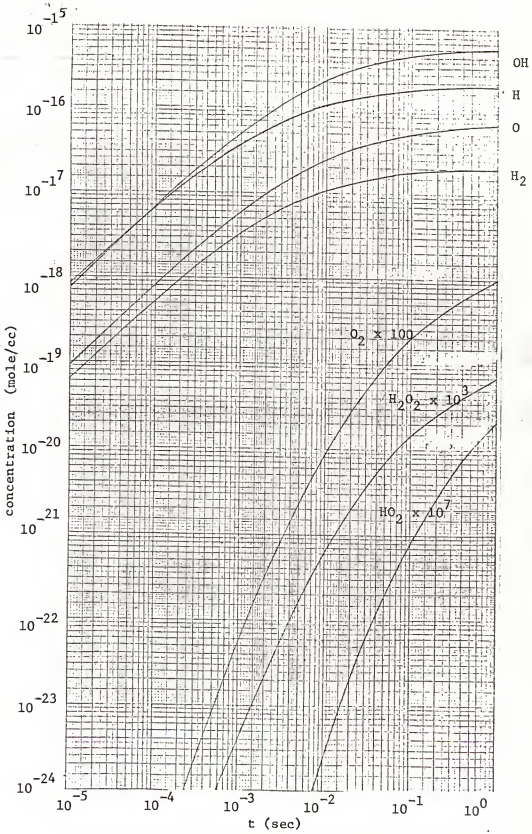

Figure 6.2. Time course at r = 0 for T = 400 K, E_o = 1 keV, n = 6 × 10^{15} #/cc and I = 10^{12} #/sec. (low density gas, slow chemistry).

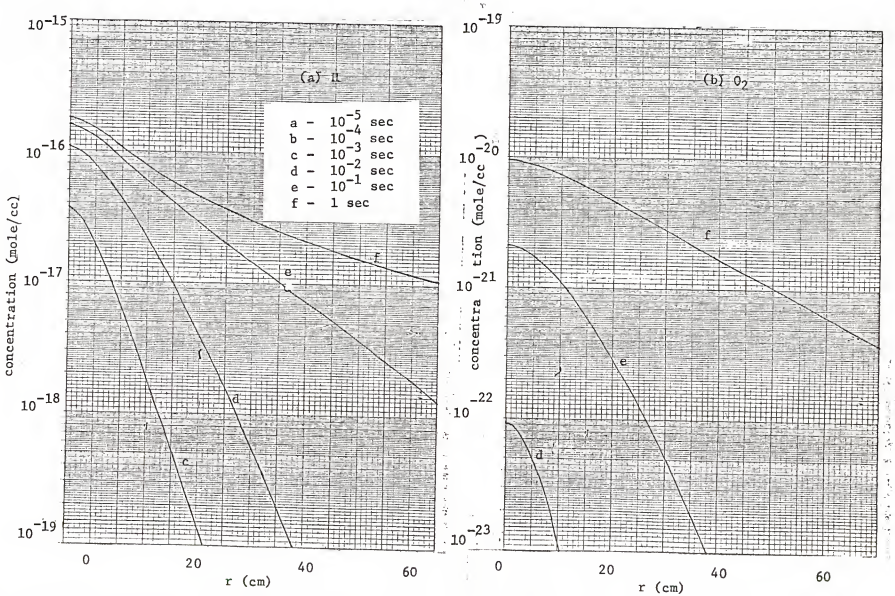

Figure 6.3. Time sequence of radial profiles for low density gas, slow chemistry case for (a) H, (b) O_2.

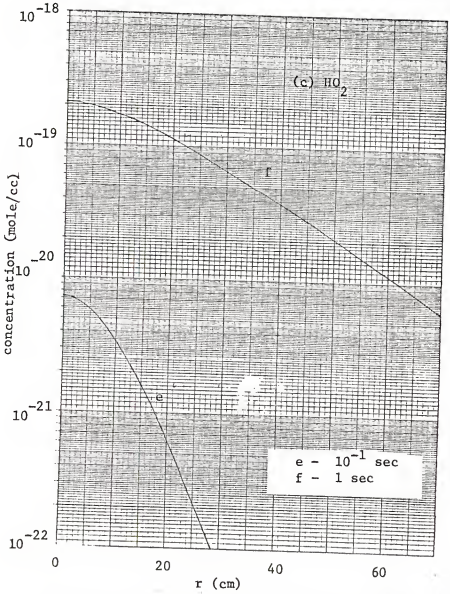

Figure 6.3. Time sequence of radial profiles for low density gas, slow chemistry case for (c) HO_2.

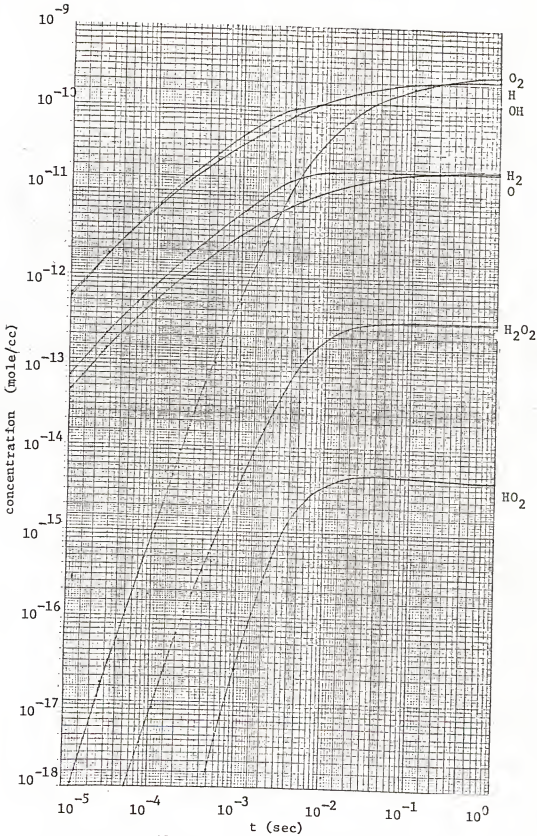

Figure 6.4. Time course at r = 0 for T = 400 K, E_o = 1 keV, $\bar{n}$ = 6 × 10^{15} #/cc and I = 10^{18} E/sec. (low density gas, borderline chemistry).

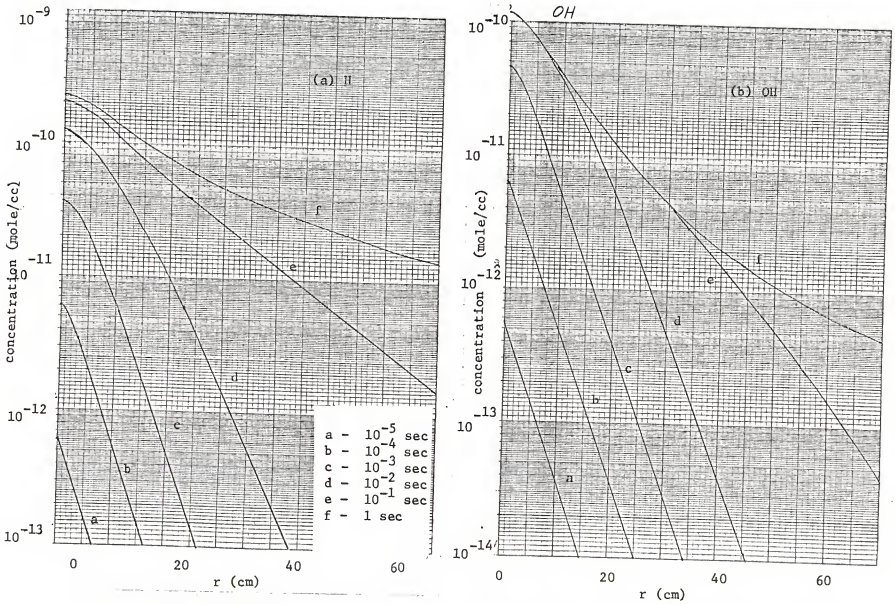

Figure 6.5. Time sequence of radial profiles for low density gas, borderline chemistry case for (a) H, (b) OH.

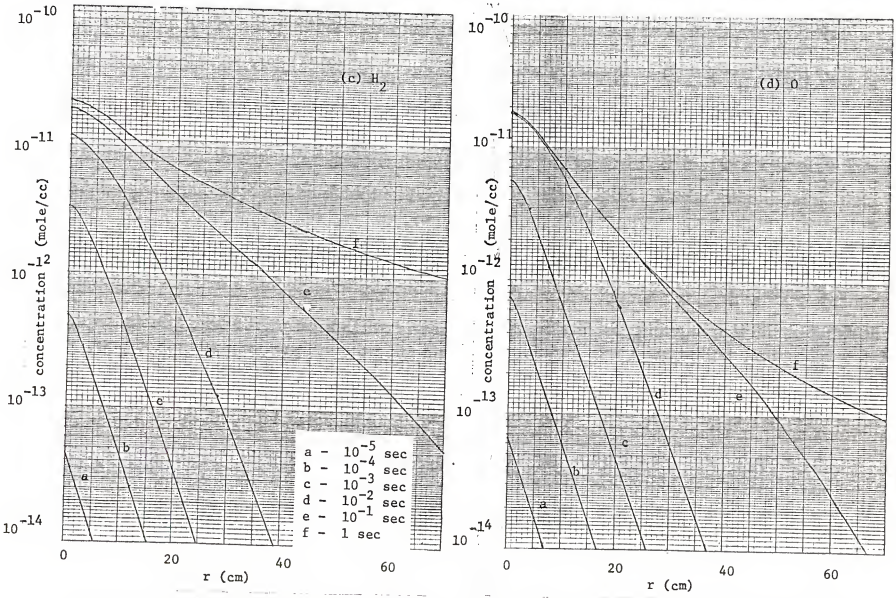

Figure 6.5. Time sequence of radial profiles for low density gas, borderline chemistry case for (c) H_2, (d) O.

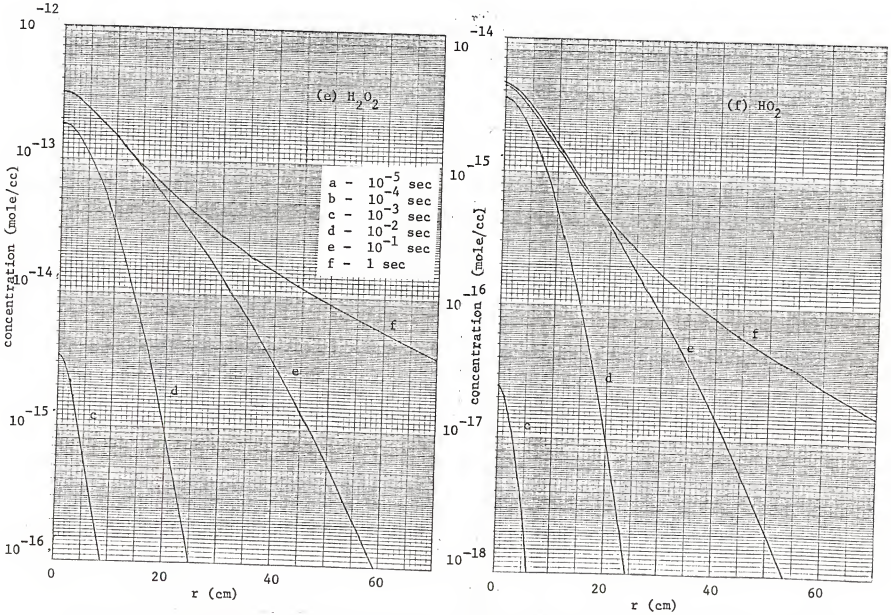

Figure 6.5. Time sequence of radial profiles for low density gas, borderline chemistry case for (e) H_2O_2, (f) HO_2.

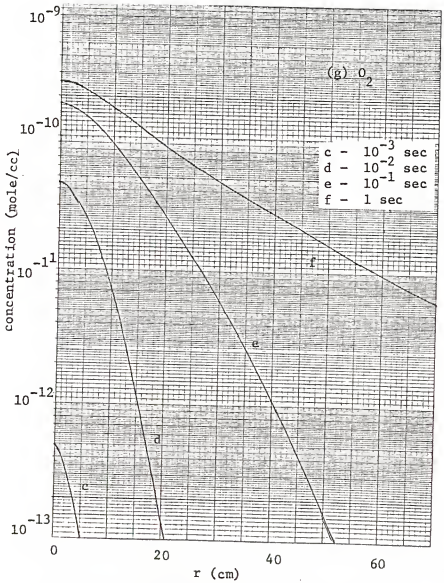

Figure 6.5. Time sequence of radial profiles for low density gas, borderline chemistry case for (g) O_2.

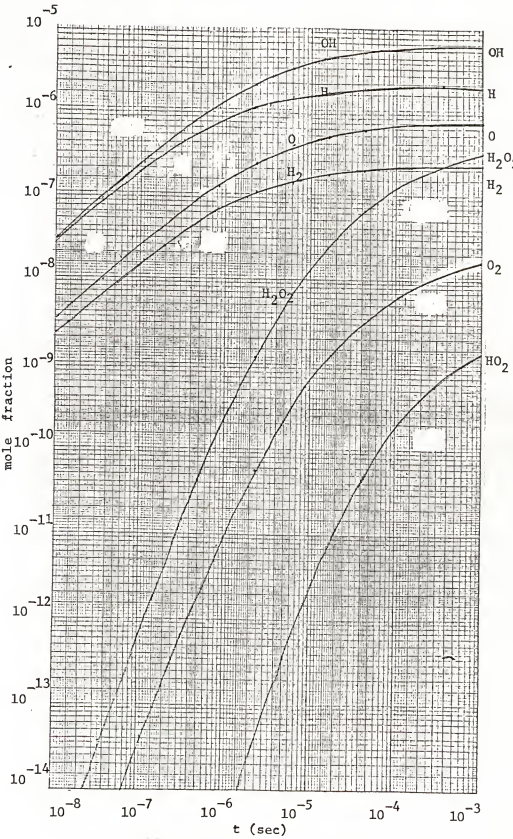

Figure 6.6. Time course at r = 0 for T = 400 K, E_o = 1 keV, n = 1.84 × 10^{19} #/cc and I^o= 3.67 × 10^{10} #/sec (1 atm gas, slow chemistry).

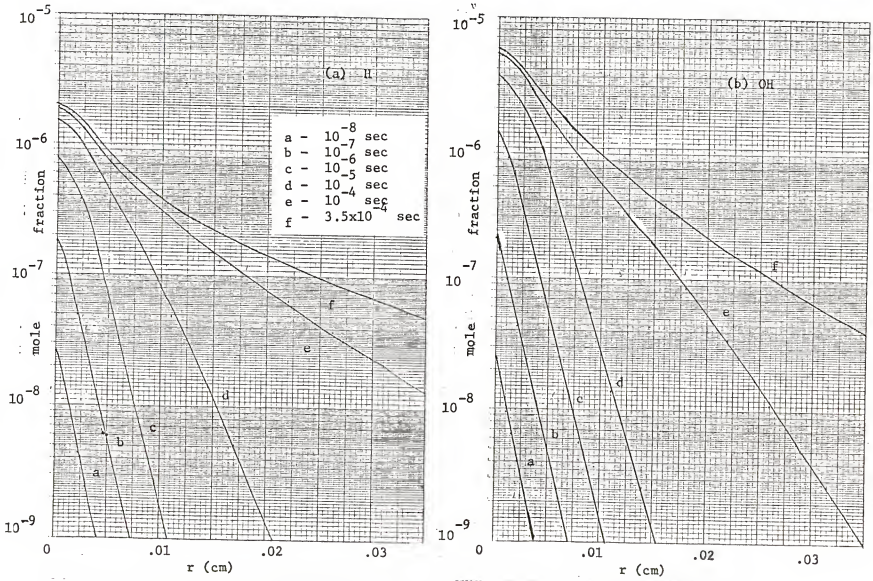

Figure 6.7. Time sequence of radial profiles for 1 atm gas, slow chemistry case for (a) H, (b) OH.

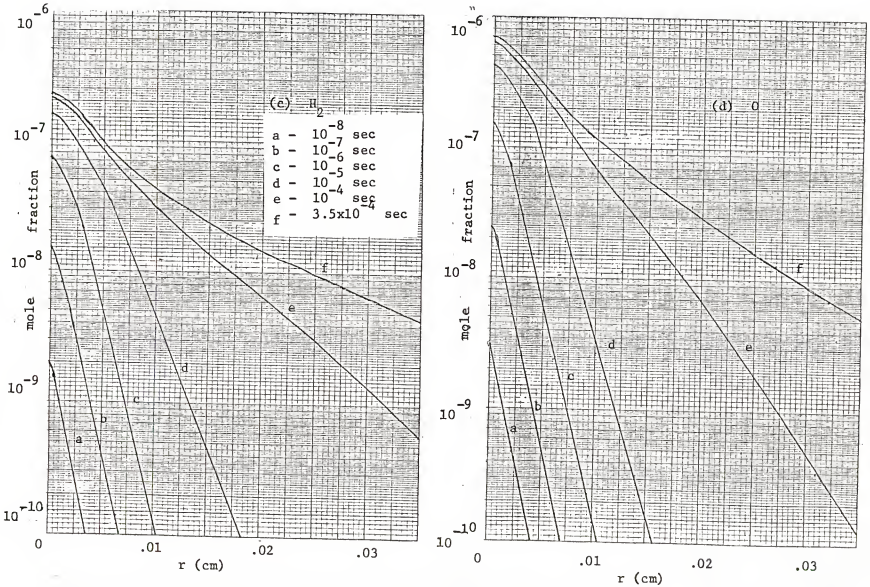

Figure 6.7. Time sequence of radial profiles for 1 atm gas, slow chemistry case for (c) H_2, (d) O.

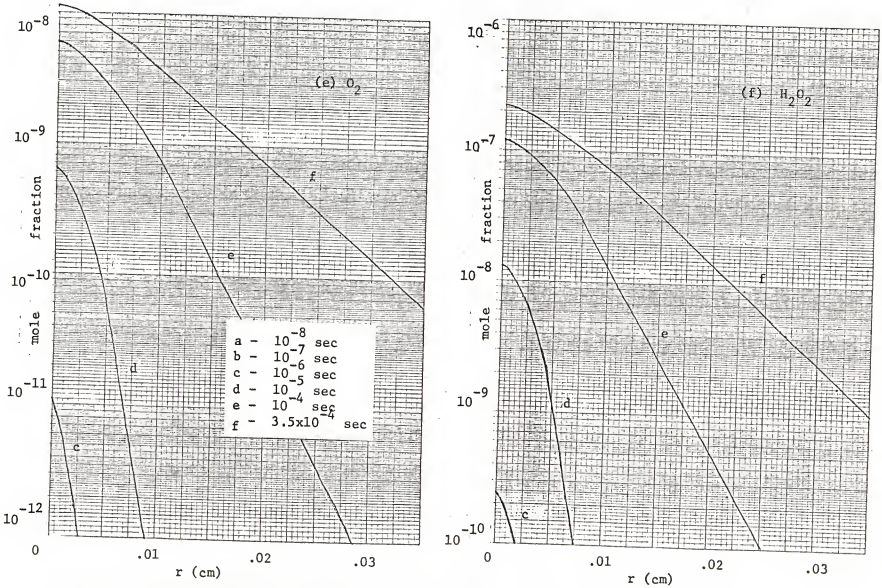

Figure 6.7. Time sequence of radial profiles for 1 atm gas, slow chemistry case for (e) O_2, (f) H_2O_2.

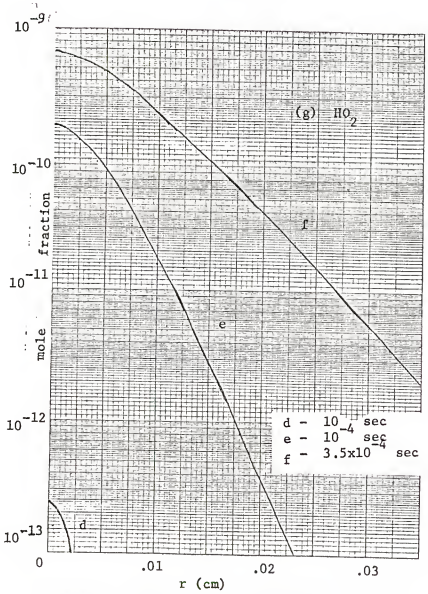

Figure 6.7. Time sequence of radial profiles for 1 atm gas, slow chemistry case for (g) HO_2.

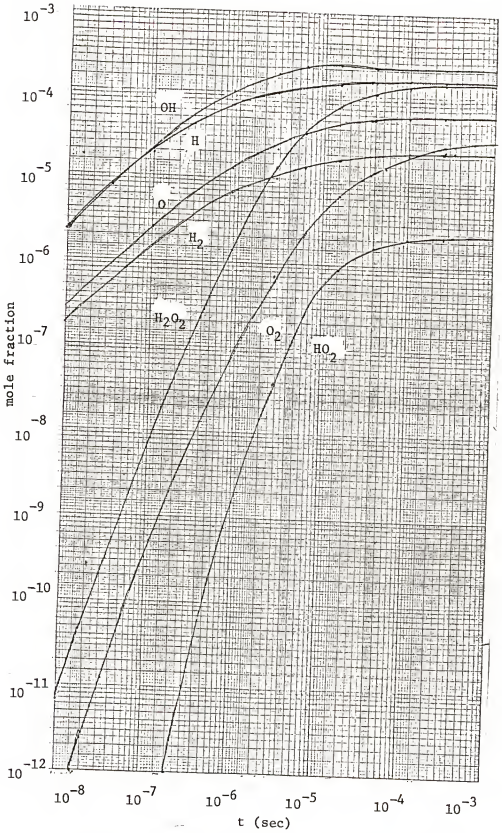

Figure 6.8. Time course at r = 0 for T = 400 K. E_o = 1 keV, n = 1.84 × 10^{10} #/cc and I^o= 3.67 × 10^{12} #/sec. (1 atm gas, borderline chemistry).

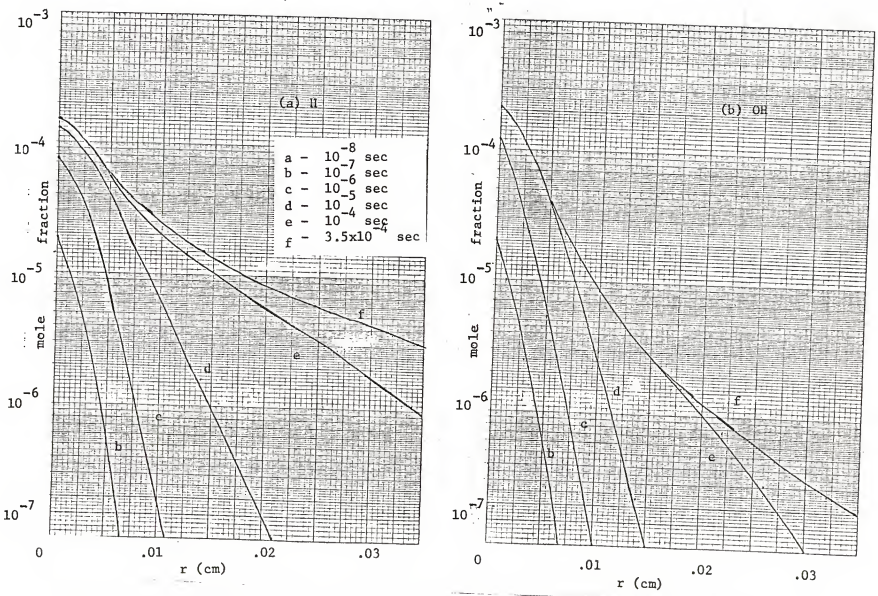

Figure 6.9. Time sequence of radial profiles for 1 atm gas, borderline chemistry case for (a) H, (b) OH.

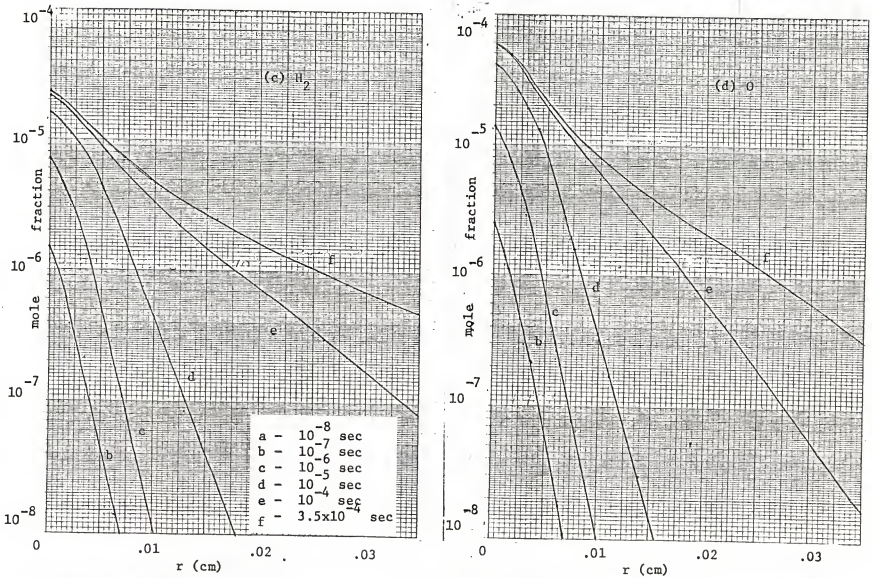

Figure 6.9. Time sequence of radial profiles for 1 atm gas, borderline chemistry case for (c) H_2, (d) O.

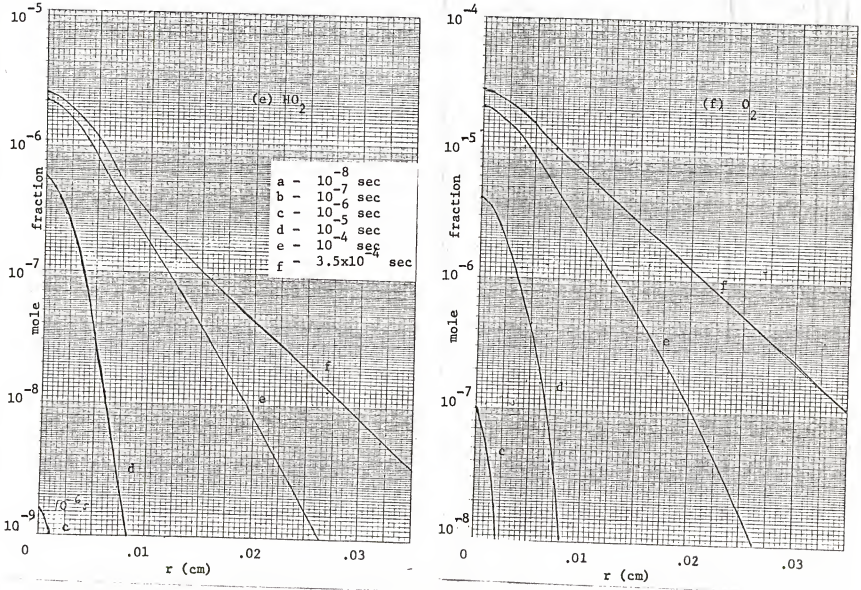

Figure 6.9. Time sequence of radial profiles for 1 atm gas, borderline chemistry case for (e) HO_2, (f) O_2.

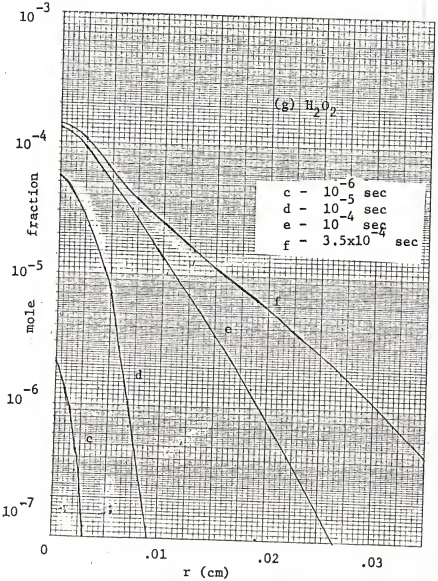

Figure 6.9. Time sequence of radial profiles for 1 atm gas, borderline chemistry case for (g) H_2O_2.

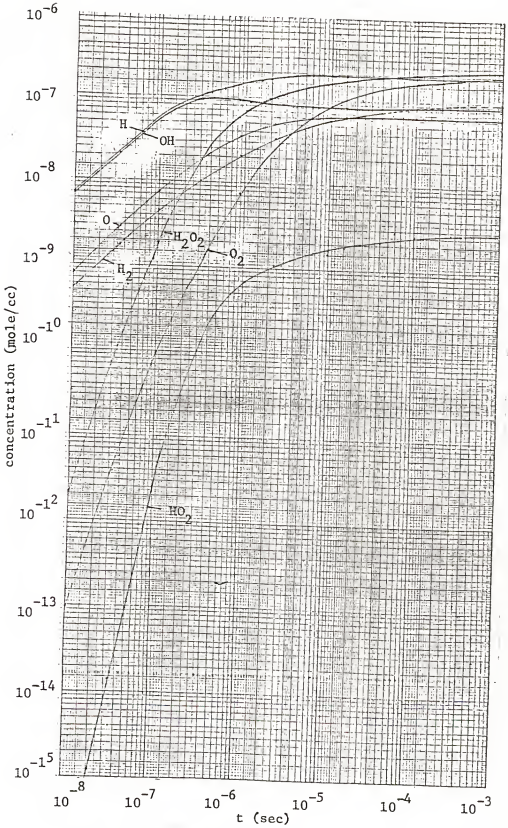

Figure 6.10. Time course at r = 0 for T_9 = 400 K, E_o = 1 keV, n = 1.84 × 10^{19} #/cc and I^o = 3.67 × 10^{14} #/sec (1 atm gas, fast chemistry).

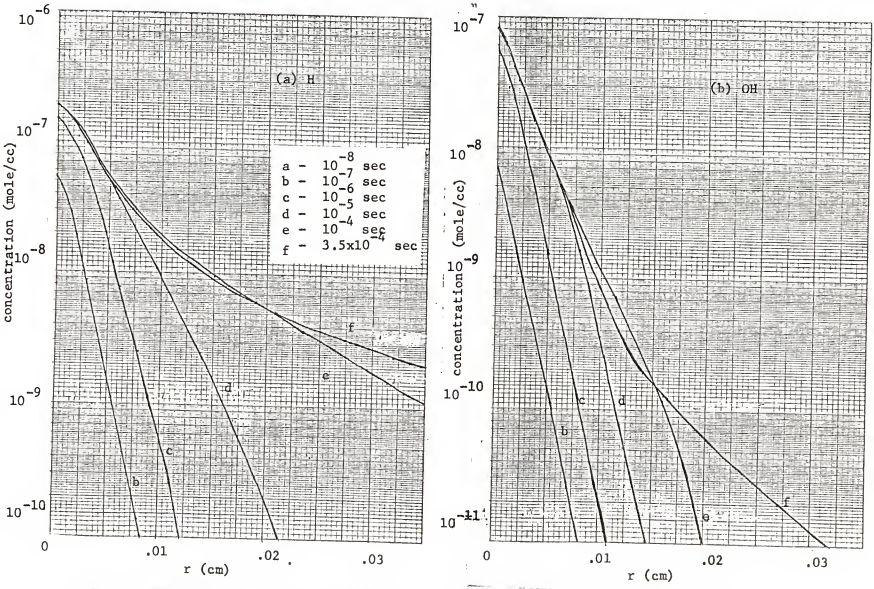

Figure 6.11. Time sequence of radial profiles for 1 atm gas, fast chemistry case for (a) H, (b) OH.

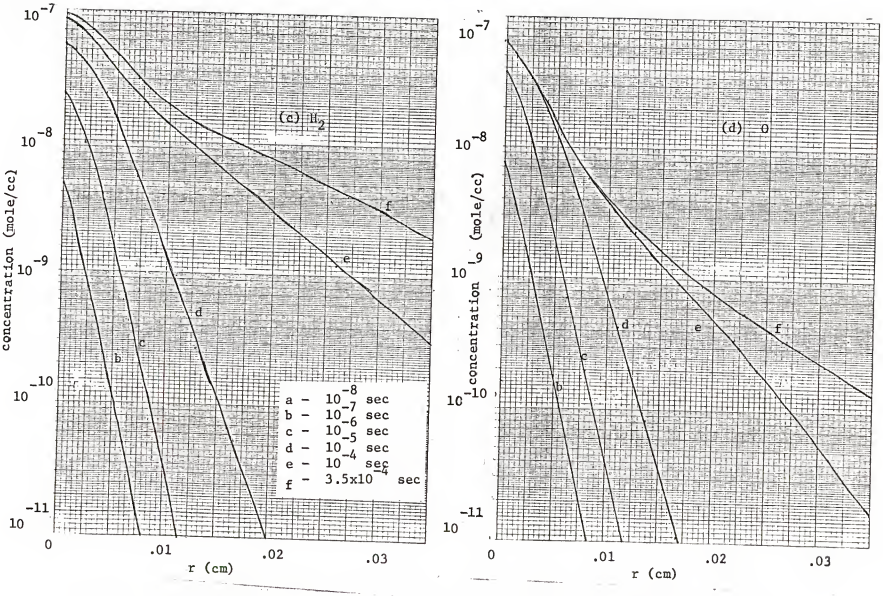

Figure 6.11. Time sequence of radial profiles for 1 atm gas, fast chemistry gas case for (c) H_2, (d) O.

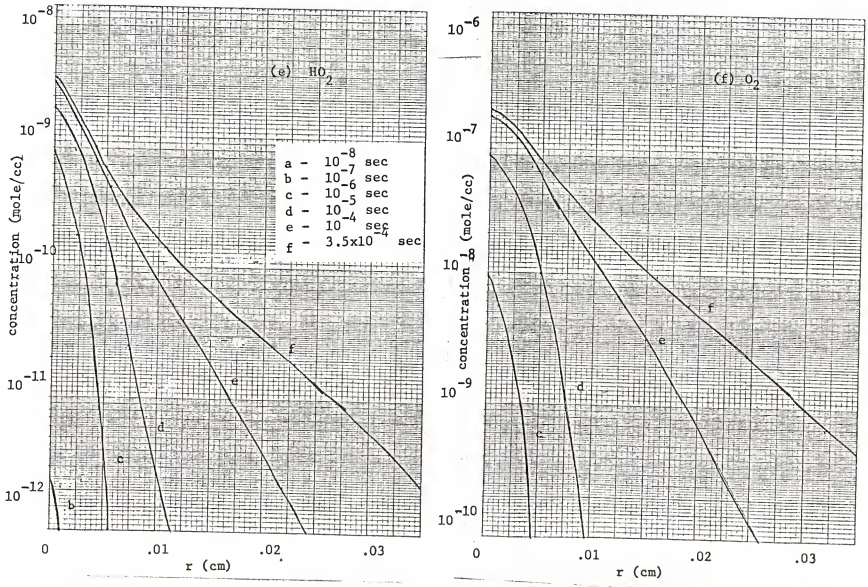

Figure 6.11. Time sequence of radial profiles for 1 atm gas, fast chemistry case for (e) HO_2, (f) O_2.

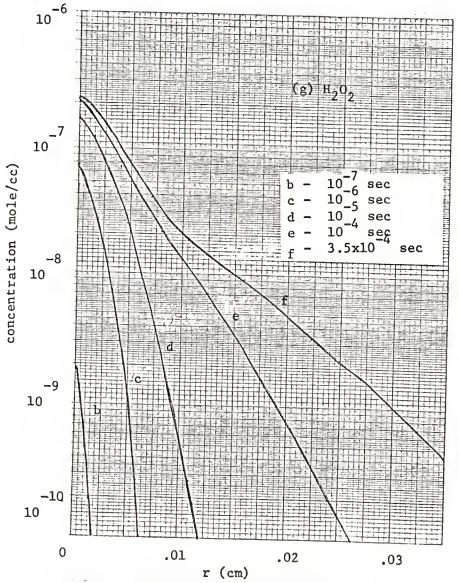

Figure 6.11. Time sequence of radial profiles for 1 atm gas, fast chemistry case for (g) H_2O_2.

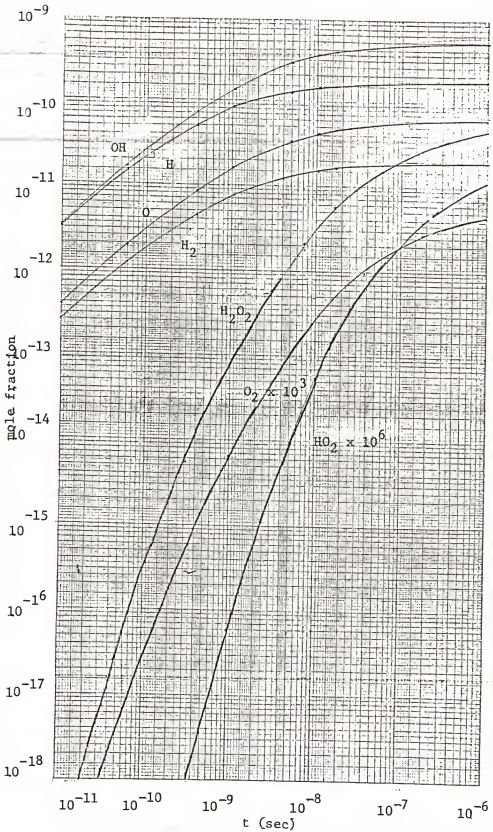

Figure 6.12. Time course at r = 0 for T = 300 K, E_o = 1 keV, n = 3.34 × 10^{22} #/cc and I^o= 1.44 × 10^3 #/sec (liquid density, slow chemistry).

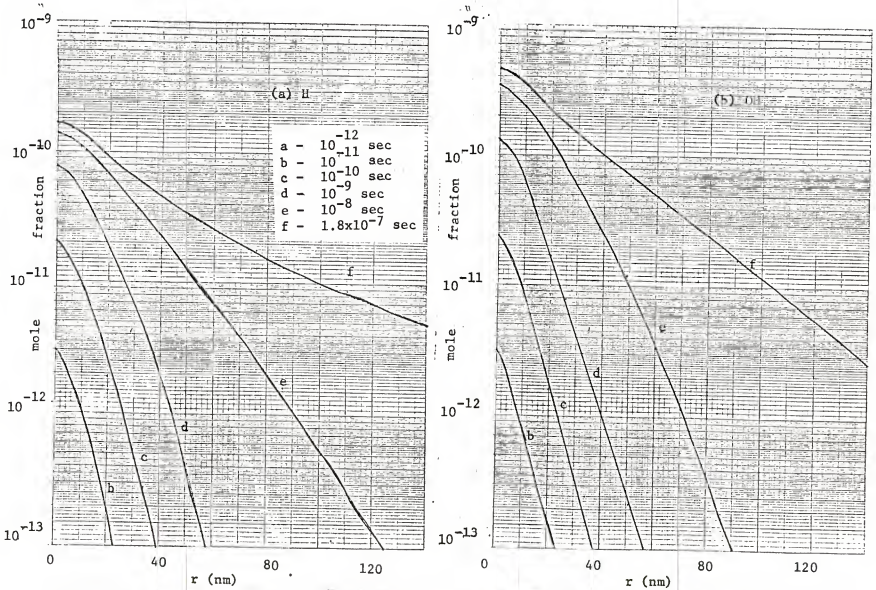

Figure 6.13. Time sequence of radial profiles for liquid density, slow chemistry case for (a) H, (b) OH.

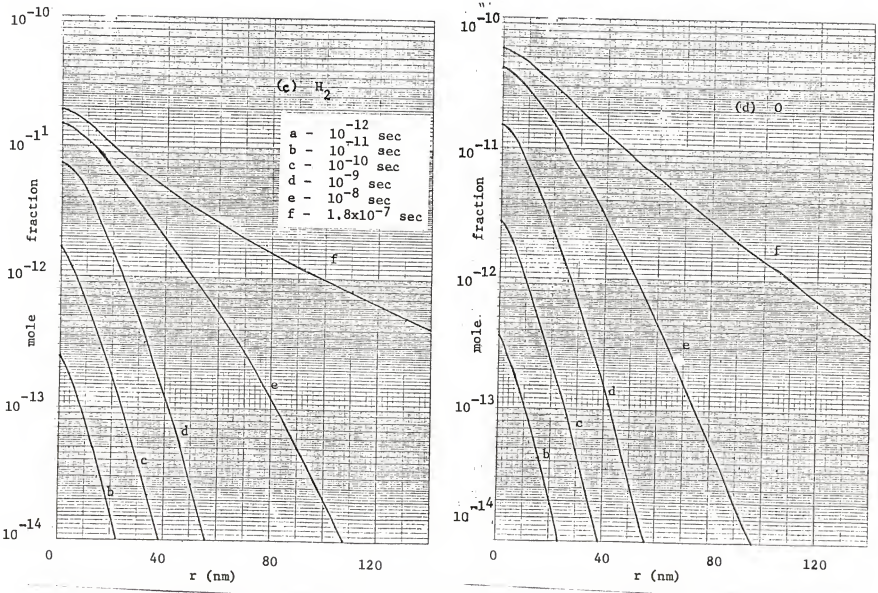

Figure 6.13. Time sequence of radial profiles for liquid density, slow chemistry case for (c) H_2, (d) O.

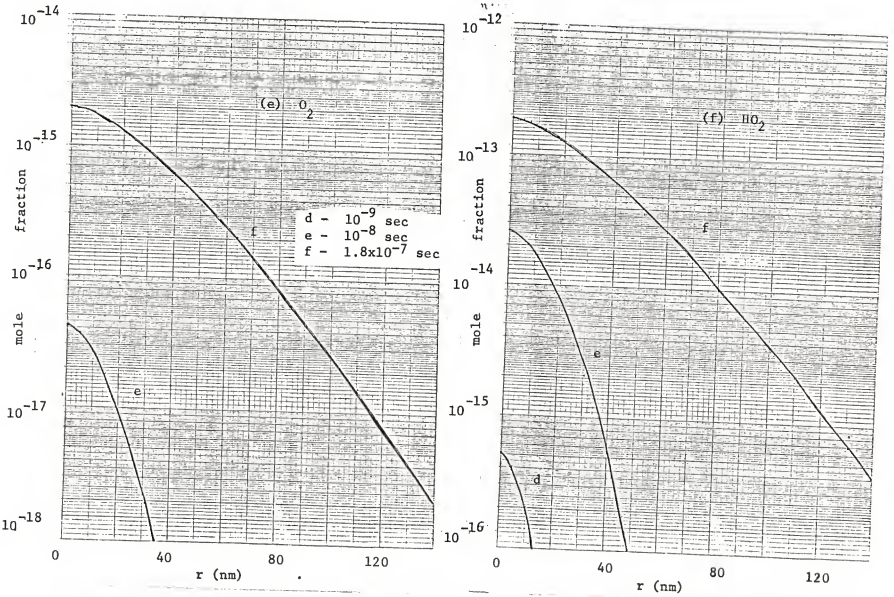

Figure 6.13. Time sequence of radial profiles for liquid density, slow chemistry case for (e) HO_2, (f) O_2.

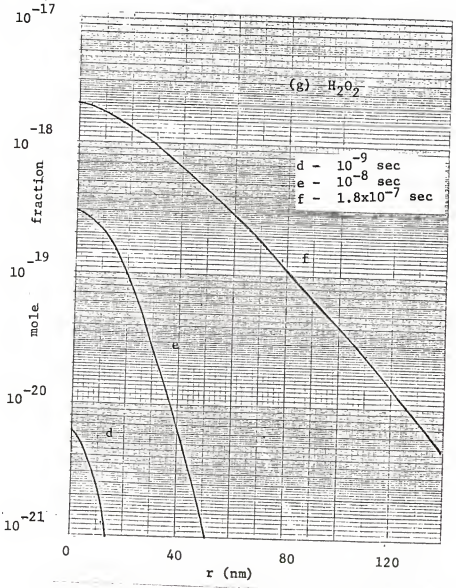

Figure 6.13. Time sequence of radial profiles for liquid density, slow chemistry case for (g) H_2O_2.

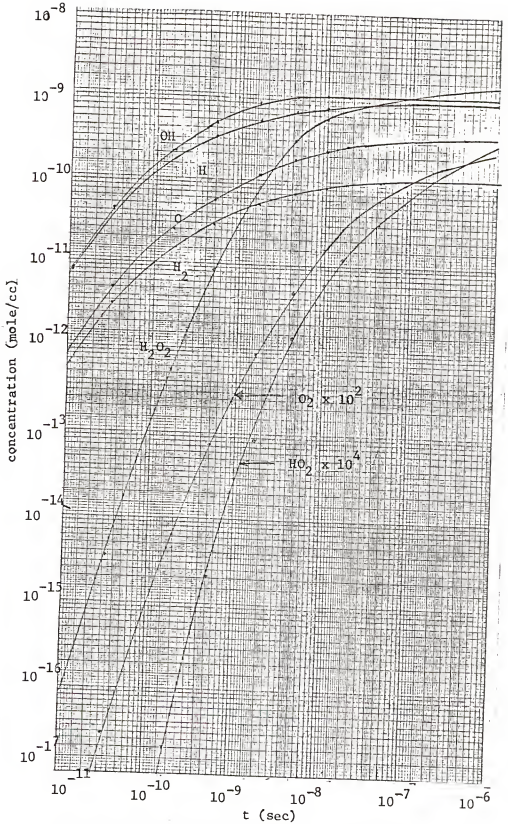

Figure 6.14. Diffusion kinetic time course at r = 0 for T = 300 K, E_o = 1 keV, n = 3.34 × 10^{22} #/cc and I = 1.44 × 10^5 #/sec (liquid density, borderline chemistry).

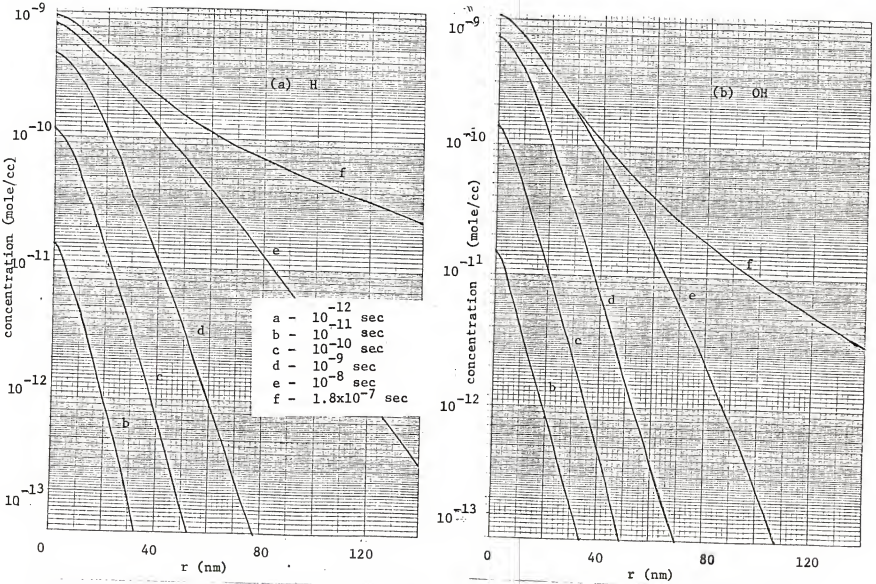

Figure 6.15. Time sequence of radial profiles for liquid density, borderline chemistry case for (a) H, (b) OH.

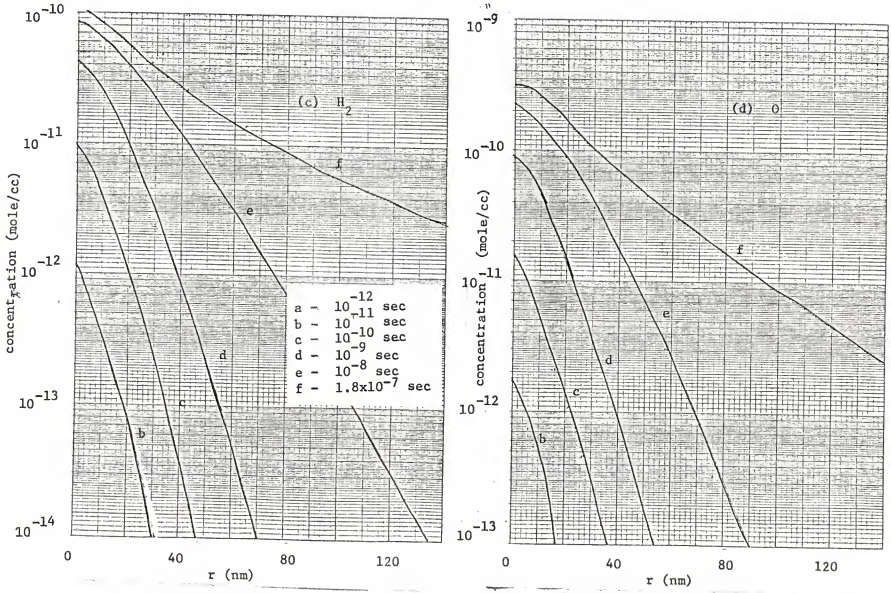

Figure 6.15. Time sequence of radial profiles for liquid density, borderline chemistry case for (c)H_2, (d) O.

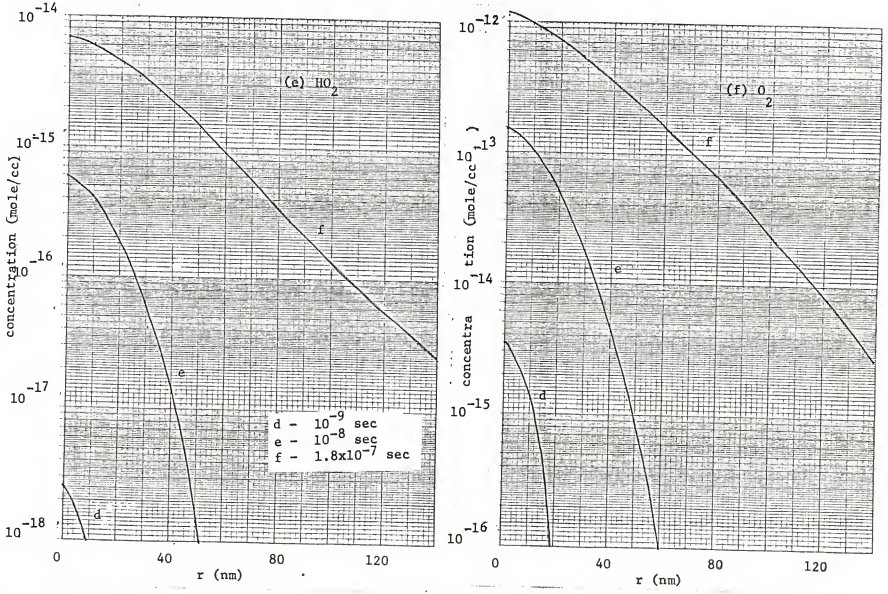

Figure 6.15. Time sequence of radial profiles for liquid density, borderline chemistry case for (e) HO_2, (f) O_2.

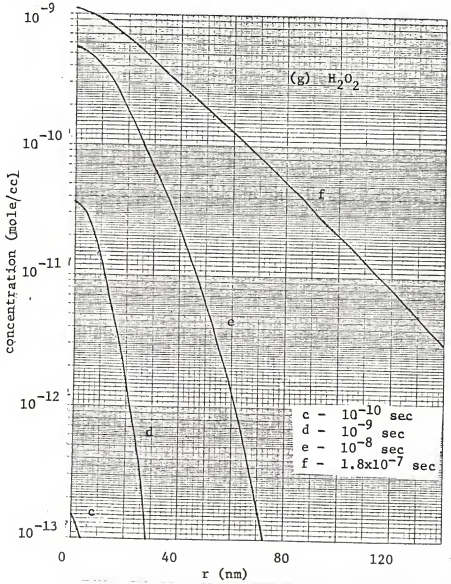

Figure 6.15. Time sequence of radial profiles for liquid density, borderline chemistry case for (g) H_2O_2.

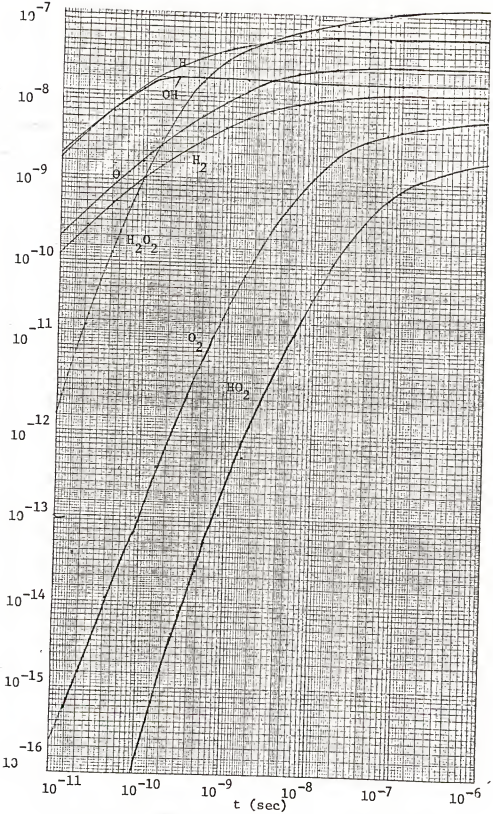

Figure 6.16. Time course at r = 0 for T = 300 K, E_o = 1 keV, n_- = 3.34 × 10^{22} #/cc and I^o = 1.44 × 10^7 #/sec (liquid density, fast chemistry).

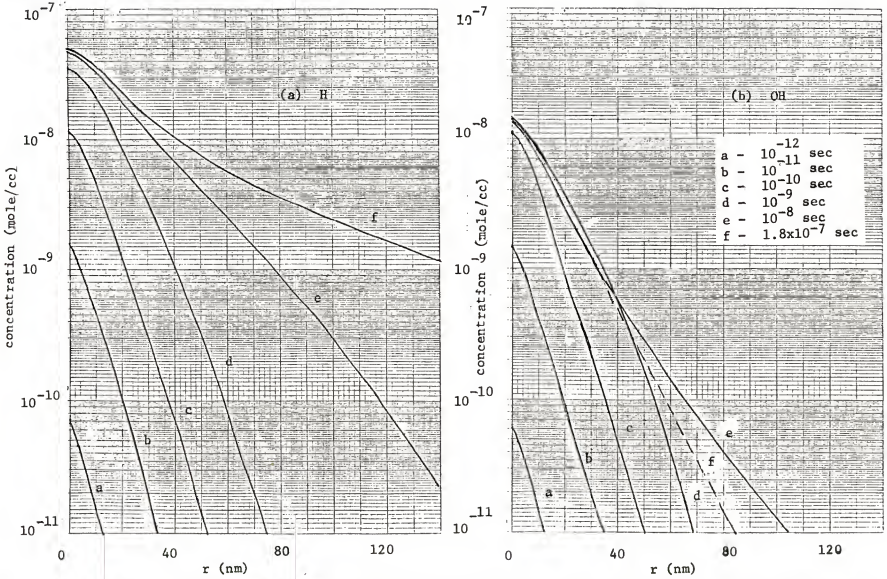

Figure 6.17. Time sequence of radial profiles for liquid density, fast chemistry case for (a) H, (b) OH.

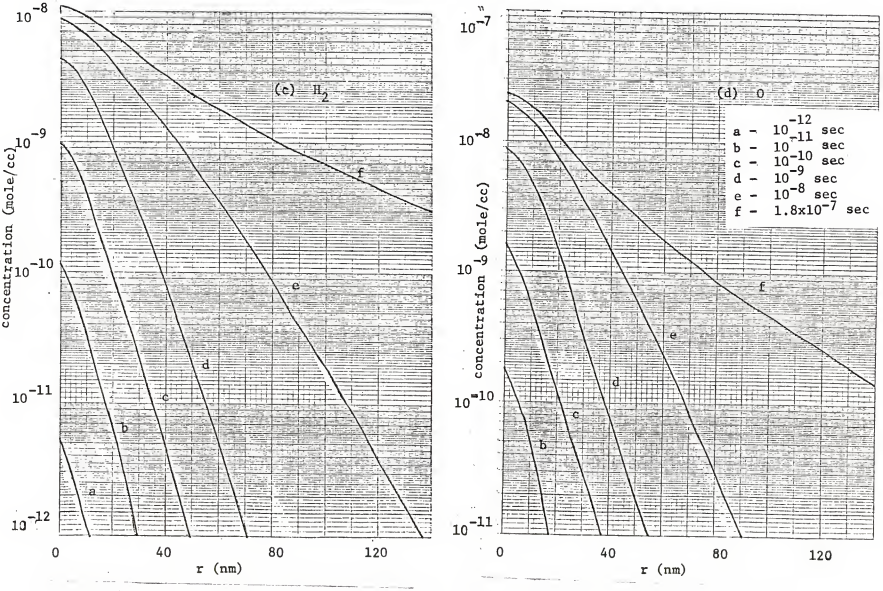

Figure 6.17. Time sequence of radial profiles for liquid density, fast chemistry case for (c) H_2, (d) O.

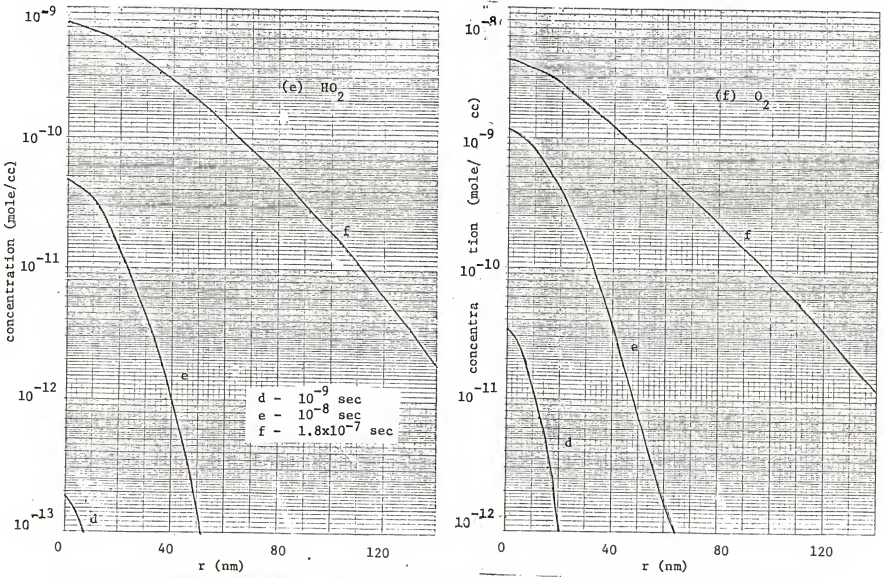

Figure 6.17. Time sequence of radial profiles for liquid density, fast chemistry case for (e) HO_2, (f) O_2.

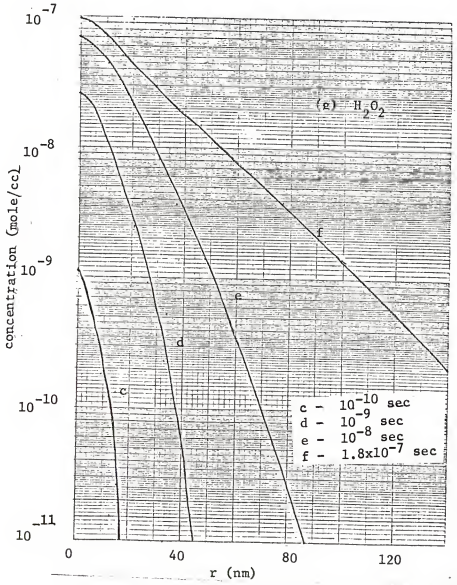

Figure 6.17. Time sequence of radial profiles for liquid density, fast chemistry case for (g) H_2O_2.

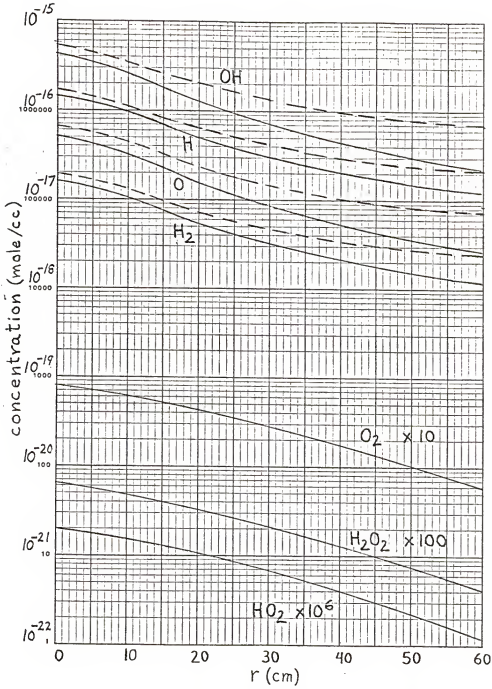

Figure 6.18. Snapshot of near steady state profiles for all species for low density, slow chemistry case, t = 1 sec. steady state pure diffusion limit overlaid for only-diffusing species.

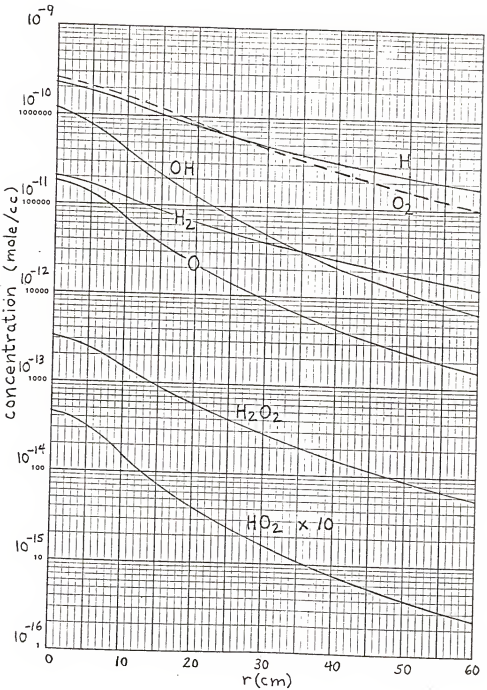

Figure 6.19. Snapshot of near steady state profiles for all species for low density, borderline chemistry case, t = 1 sec.

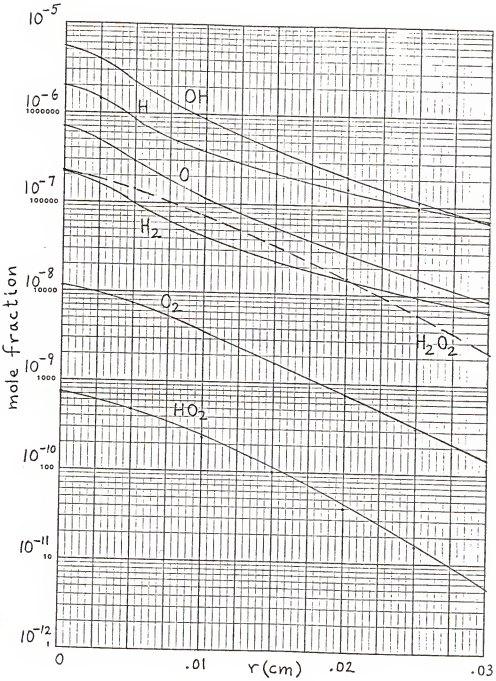

Figure 6.20. Snapshot of near steady state profiles for all species for 1 atm, slow chemistry case, $t = 3.5 \times 10^{-4}$ sec.

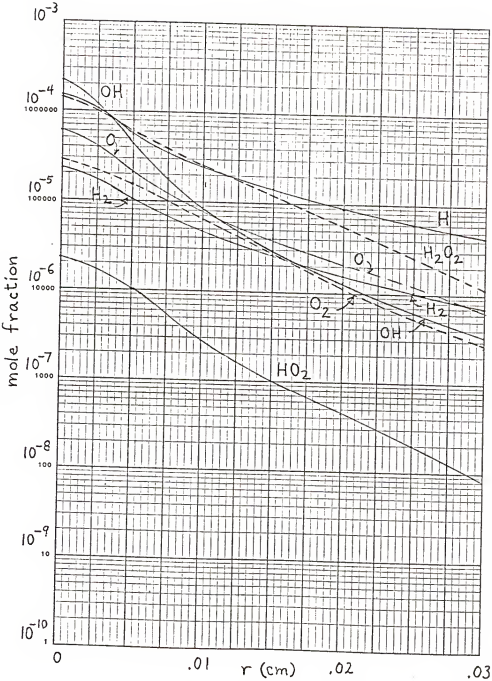

Figure 6.21. Snapshot of near steady state profiles for all species for 1 atm, borderline chemistry case, $t = 3.5 \times 10^{-4}$ sec.

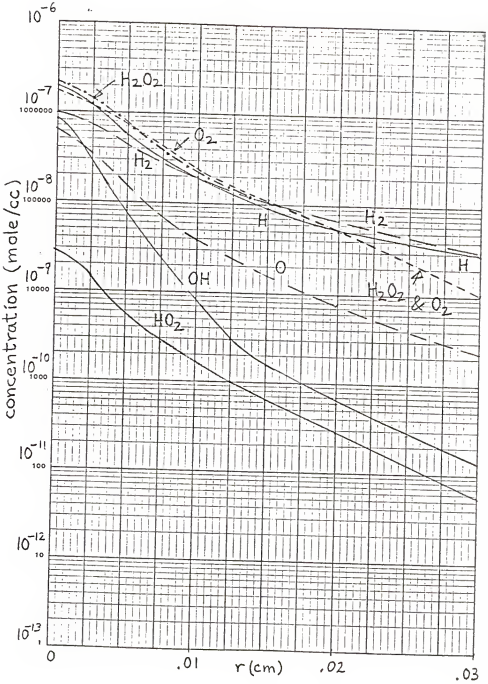

Figure 6.22. Snapshot of near steady state profiles for all species for 1 atm, fast chemistry case, $t = 3.5 \times 10^{-4}$ sec.

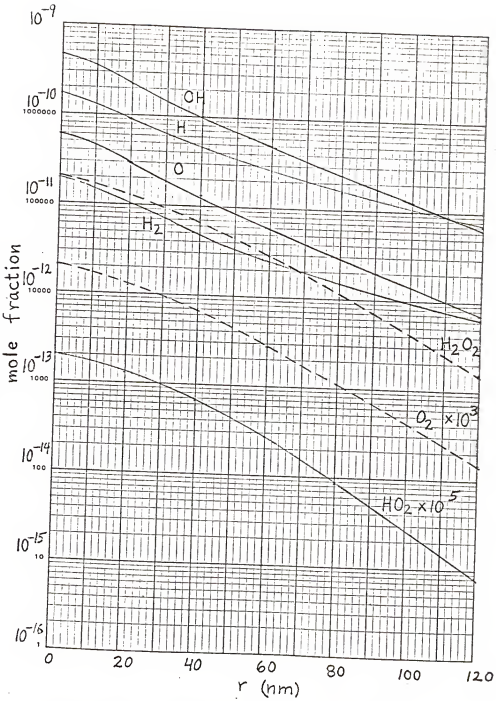

Figure 6.23. Snapshot for near steady state profiles for all species for liquid density, slow chemistry case, $t = 1.8 \times 10^7$ sec.

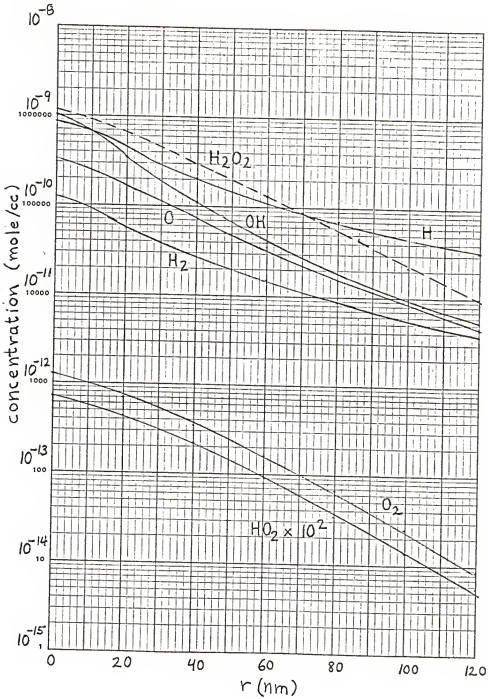

Figure 6.24. Snapshot of near steady state profiles for all species for liquid density, borderline chemistry case, $t = 1.8 \times 10^{-7}$ sec.

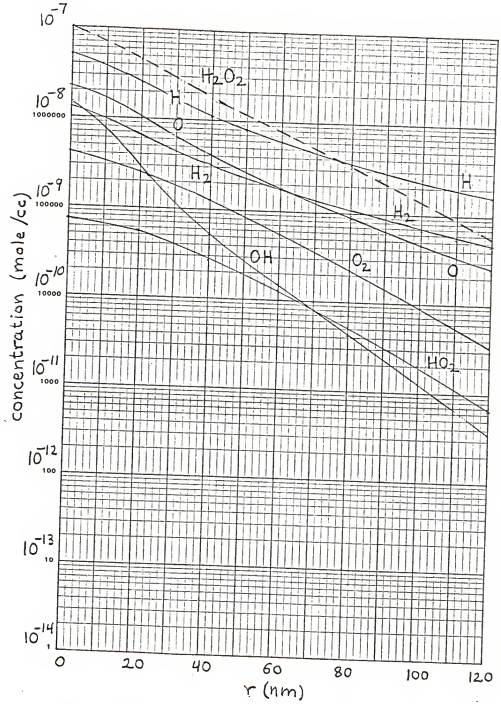

Figure 6.25. Snapshot of near steady state profiles for all species for liquid density, fast chemistry case, $t = 1.8 \times 10^{-7}$ sec.

reaction time and diffusion time; (2) fundamental diffusion kinetic results for single body decay and for both one and two species two body decay, presented in Chapter III; (3) time dependent diffusion results, for example, diffusion time, but more extensively, the Green's function approach in the late chemistry case; (4) and so on.

In summary, it seems fair to note that this alternate mode of presentation of the results has enabled us to draw one very significant conclusion which would probably have escaped us otherwise. This mode can properly be said to complement the modes of presentation implemented up to this point.

Energy Dependence

It would be useful to form an idea of the dependence of the diffusion kinetics trends in g and h, equivalently in i and h, on incident energy, E_o. In Chapter II we concluded that the spatial yields could be represented by the form

$$y_i(\rho,z) = A_{io,s}(E_o)\, e^{-\beta_{o,s}(E_o)d\xi} + A_{i2,d}(E_o)\, e^{-\beta_{2,d}(E_o)d\xi} \tag{6.1}$$

where

$$A_{ij}(E_o) = [\beta_j^3(E_o)d^3\gamma^2(E_o)(1-\varepsilon^2(E_o))^2/8\pi](g_{ij}(E_o)E_o/100)I \tag{6.2}$$

and

$$\xi = \sqrt{\gamma^2(E_o)\rho^2 + (z - z_o(E_o))^2} - \varepsilon(E_o)(z - z_o(E_o)) \tag{6.3}$$

where $z_o(E_o) = z_o'(E_o)/d$.

It was also found that a reasonably equivalent concentric form (i.e., one for which $\varepsilon = 0$) could be constructed by making the transformations

$$\begin{aligned} \varepsilon &\to \varepsilon_{con} = 0 \\ \gamma &\to \gamma_{con} = \gamma \\ \beta &\to \beta_{con} = \beta(1 - \varepsilon^2)^{2/3} \end{aligned} \tag{6.4}$$

and adjusting z_o' by nonlinear least squares fit. From this concentric form an equivalent spherical form is found at once by making the transformations

$$\begin{aligned} \varepsilon_{con} = 0 &\to \varepsilon_{sph} = 0 \\ \gamma_{con} &\to \gamma_{sph} = 1 \\ \beta_{con} &\to \beta_{sph} = \gamma^{2/3}\beta_{con} \\ z'_{o,con} &\to z'_{o,sph} = z'_{o,con} \,. \end{aligned} \tag{6.5}$$

The form of $y(\rho,z)$ now simplifies to

$$y_i(r) = A_{io,s}(E_o)e^{-\beta_{o,s}(E_o)dr} + A_{i2,d}(E_o)e^{-\beta_{2,d}(E_o)dr} \tag{6.6}$$

where $r = \sqrt{\rho^2 + (z - z_o)}$.

The question of what to do with this double exponential form, considering that the development of all of our diffusion kinetic results so far has been based on a single exponential form for the source terms, stands now in our way. In either extreme, where one of the two exponentials, the short range or the long range, vastly predominates over the other, the problem is solved--the source term effectively degenerates to a single exponential. The ratio, $\beta_{io,s}/\beta_{i2,d}$, approaches a maximum value of 4.4 (recall k = 4.4 in Eq. (2.29)) as E_o decreases, and approaches a minimum value of 1 as E_o increases. The ratio $g_{io,s}/g_i$ approaches a maximum value of 1 as E_o decreases, and a minimum value of about 0.1 as E_o increases. For $E_o \gtrsim$ 1keV the short range term can be neglected, while for $E_o \lesssim$ 300 eV the long range term can be neglected. In between, we may approximate matters by a single exponential for which β is assigned some intermediate value between the two extreme limits. Since this assignment is an estimate, a confidence interval should be assigned along with it.

The interesting quantities whose dependence on E_o we would like to identify are τ_d and τ_c. Let us first consider τ_d. The diffusion time, τ_d, is given by by $1/D_o d_o \beta^2(E_o)h$. It is proportional to the square of the range of the deposition, and therefore increases with increasing E_o. In the Born limit, it therefore goes as $E_o^{3.5}$. The reaction time, τ_c, is given by

$$\tau_c = \begin{cases} \dfrac{1}{\sqrt{k_{1b}((g_{OH}(E_o) - g_O(E_o))/100)E_o(\beta^3(E_o)d^3 I/8\pi)}}, & d < 4.6(-4)\ \text{gm/cc} \\[2ex] \dfrac{1}{\sqrt{k_{6b}(g_{OH}(E_o)/100)E_o(\beta^3(E_o)d^3 I/8\pi)C_{H_2O}}}, & d > 4.6(-4)\ \text{gm/cc} \end{cases} \tag{6.7}$$

or, equivalently in terms of g and h, by

$$\tau_c = \begin{cases} \overline{1/\sqrt{k_{1b}((g_{OH}(E_o) - g_o(E_o))/100)E_o(\beta^3(E_o)d_o{}^3I_o/8\pi)g}}, & h < 256 \\ \overline{1/\sqrt{k_{6b}(g_{OH}(E_o)/100)E_o(\beta^3(E_o)d_o{}^3I_o/8\pi)(d_o/18.021)gh}}\ , & h > 256\ . \end{cases} \tag{6.8}$$

For $E_o > 200$ eV the g-values are nearly constant. E_o dependence comes in through the factor of E_o and from $\beta(E_o)$. In the Born limit, it therefore goes as $E_o{}^{2.1}$. The reaction time is therefore seen to increase much more slowly with E_o than the diffusion time. All other things being equal, the chemistry becomes progressively earlier, in fact much earlier, as the incident energy of the electron beam is increased.

For very high incident energy, the contours of deposition become more and more singly confocal, so that a concentric approximation, let alone a spherical one, becomes less and less adequate. The problem then becomes irreducibly two dimensional.

In the extreme limit, the geometry of the problem approaches that of a cylinder, which is also one-dimensional--specifically, a a cylinder with a bulb on the end where the electron and its high energy secondaries have significantly slowed down, and are giving rise to many low energy secondaries. At not such extreme high energy limit (relativistic), this bulb engulfs the narrow core or stem of higher energy electrons which give rise to it, resulting in the contours we have calculated at 10 keV (see Fig. 2.10), and which Grün (1956) and

Cohn and Caledonia (1970) report at incident energies of from 5-54 keV and 2-5 keV, respectively. In Chapter II we have referred to this configuration as 'penumbra' and 'core.'

Let us consider for a moment such a plume shape in detail before going on. It is characterized by a forward and a backward fall off, $\beta_f(E_o) = \beta(E_o)(1 - \varepsilon(E_o))$ and $\beta_b(E_o) = \beta(E_o)(1 + \varepsilon(E_o))$. Because $\gamma(E_o) \sim \sqrt{1 - \varepsilon^2(E_o)}$ for high E_o, the fitted contours are nearly circular (this is a simplified approximation in the central core) about a common 'affine focus'. The geometry of the backplume is something in between a nearly flat lens-like shape and a hemisphere half-centered on the 'affine focus.' The forward plume resembles a somewhat deformed sphere.

The sphericalization of the entire form (see above) more strongly resembles the forward plume. This reflects the relative sizes of these two regions. From Eqs. (6.4) and (6.5) it follows that the sphericalized fall off, β_{sph} is equal to $\beta(1 - \varepsilon^2)$, which lies in between the forward fall off, $\beta(1 - \varepsilon)$, and the backward fall off, $\beta(1 + \varepsilon)$, but closer to the forward.

This essay in estimation has been presented in order to lay a foundation for a future link-up of the spherical form source term diffusion kinetic results obtained here and future work with source terms of more general shape. Such future work is seen as a possibility via an upgrading of DIFKIN to calculate for a generalized polar as well as generalized radial grid. Specifically, the affine singly confocal coordinate system, or even a more general radial-type coordinate system, is seen as the most useful route to take for this purpose.

Heating Effects

In the radiological problem addressed in this work certain physical assumptions have been made. The first of these is that the system remains dilute, in other words, that a steady, uniform background of H_2O be maintained. This is necessary, in the first place, because the calculation of the spatial yields is based upon this assumption. It is necessary, in the second place, because, should it not be the case, then, because of the law of partial pressures, a convective regime will be set up, which contradicts the assumption of the diffusion kinetic equations, that the medium is stagnant. The "depletion time," defined in Chapter V, can serve to identify an upper limit on injection rate mandated by this requirement. Of the eight hypothetical cases considered, one, the high injection rate case for low density gas lies dangerously near this limit. In this case, H_2O level is down to 94.6% at r=0 at 0.1 sec, and 92.8% at 1 sec. In all the other cases, H_2O depletion is negligible.

A yet more severe limit, the upper limit on injection rate due to heating, must next be addressed. A full treatment of this problem would have to take into account the energetics of the chemical reactions. In lieu of this, a rough order of magnitude estimate is made here, arguing from conservation of energy and the equipartition theorem.

The time rate of energy delivered to the system, or power input to the system, is given by $P = IE_o$. In lieu of a more involved statistical mechanical derivation, as an order of magnitude estimate we may set

$$p(r) = IE_o(\beta^3 d^3/8\pi)e^{-\beta dr}. \tag{6.9}$$

Dividing by 7nk/2, where n, as used before, is the number density (assigning 3kT/2 for kinetic energy, kT for vibrational, and kT for rotational energy), one obtains a spatially distributed heat source, $y_{th}(r)$, as follows:

$$y_{th}(r) = IE_o(\beta^3 d^3/8\pi)e^{-\beta dr}/(7nk/2)$$

$$= \left(\frac{I_o d_o^2 m_{H_2O}}{28\pi N_o k}\right)\cdot E_o\beta^3(E_o)\cdot h^2 i\cdot e^{-\beta dr}$$

$$= 0.4\ (^oK/sec)\ (E_o/1\ keV)[\beta(E_o)/\beta(1\ keV)]^3\cdot h^2 i \qquad (6.10)$$

Here m_{H_2O} is the gram-molecular weight of H_2O.

Taking into account thermal conductivity of the medium, the heat equation, or thermal diffusion equation,

$$\frac{\partial T}{\partial t} = \frac{K}{c_{p_{H_2O}}\ C_{H_2O}}\ \nabla^2 T + y_{th}(r,t) \qquad (6.11)$$

follows, where $c_{p_{H_2O}}$ is molar specific heat, C_{H_2O} is molar density, $T = T(r,t)$ is temperature, and temperature dependence of the thermal conductivity, K, has been neglected. Noting that $K = K_o(T/T_o)^q$ where $q = 1.83$ and $T_o = 273^oK$ and $K_o = 3.61\times10^{-5}$ cal/gm/cm/sec/^oK for steam (Kanury, 1975), and recalling the formula for diffusion time from Chapter III, we obtain

$$\tau_{th} = c_{p_{H_2O}} C_{H_2O}/K\beta^2 d^2 = .0038\ (T/T_o)^q/h \text{ sec} \quad \text{(vapor)} \tag{6.12}$$

The equivalent diffusion coefficient differs on the low side of the diffusion coefficient of H_2O due to effects of nonmonatomic gas. For liquid water, the still lower value, K = .00146 cal/gm/cm/sec/^oK at 300^oK (CRC Handbook, 1975), reflecting collective effects.

Recalling the definition of diffusion time, it follows that $T_f = T(r=0,\infty)$ is given by

$$\begin{aligned} T_f &= y_{th}(r=0)\tau_{th} \\ &= (0.4h^2 i)(.0019/h)\ ^oK \\ &= 0.00076hi\ (^oK). \end{aligned} \tag{6.13}$$

The values of T_f which follow from Eq. (6.13) for the eight cases considered are given in Table 6.3. These values should only be taken as order of magnitude estimates, and could be wrong on either the low or the high side. All the same, we are led to conclude that two and possibly three of the cases considered are physically ruled out as a result of overheating. (In these two cases, the significance of the estimate is only that the temperature increase is too large. For such a strong heating effect, the T dependence of K, along with convective effects of thermal expansion, invalidate Eq. (6.11).) Still, something has been gained by considering them insofar as our understanding of the behavior of diffusion kinetic systems in general. For example, the character of results for the isolated H + OH system considered in

TABLE 6.3
Rough Estimate of Heating Effects of Electron Beam

case	n (#/cc)	I (#/sec)	h	i	g	est $T_f(r=0)$ (^oK)
1	6.(15)	1.(12)	1	1	1	0.0008
2	6.(15)	1.(18)	1	1.(6)	1.(6)	800.
3	1.84(19)	3.67(10)	3067.	0.0367	1.06(9)	0.045
4	1.84(19)	3.67(12)	3067.	3.67	1.06(11)	4.5
5	1.84(19)	3.67(14)	3067.	367.	1.06(13)	450.
6	3.34(22)	1.44(3)	5.56(6)	1.44(-9)	2.48(11)	4.(-7)
7	3.34(22)	1.44(5)	5.56(6)	1.44(-7)	2.48(13)	4.(-5)
8	3.34(22)	1.44(7)	5.56(6)	1.44(-5)	2.48(15)	0.004

$h = d/d_o = n/n_o$ where $n_o = 6.(15)$ #/cc
$i = I/I_o$ where $I_o = 1.(12)$ #/sec
$g = ih^2$

$$T_f(r=0) = y_{th}(r=0)\tau_{th} = (.4g/h)(.002/h) = .0008g/h^2$$
$$= (.4ih^2)(.002/h) = .0008ih$$

for ambient T = 400 ^oK, vapor

$$= (.4g/h)(.000094/h) = .000038g/h$$
$$= (.4ih^2)(.000094/h) = .000038ih$$
$$= .122(-17)g$$
$$= 209i$$

for ambient T = 300 ^oK, liquid (h = 5.56(6))

Chapter III remain essentially unchanged in going over to the physically more realistic system in the liquid state--only spatial and temporal scales would be changed.

CHAPTER VII
DISCUSSION AND CONCLUSION

Comparison with Results of the Steady State Code, DIFKT

The work embodied in this thesis was originally envisaged as a backup approach to a parallel effort to calculate steady state diffusion kinetics for the same inputs, namely, the Ph. D. thesis work of Rio (1983). That work however remains in a comparatively rough state of development. As a result of continuation of this steady state diffusion kinetics work by collaborative effort within this group, Dr. Dayashankar, Professor Green and the author, certain numerical difficulties of the code have come to light. These problems include:

(1) In assorted checks devised to test the accuracy of this code for simple problems of pure diffusion, diffusion kinetics of single body decay of one species, and of two body decay of one or two species, the code has shown unacceptable levels of inaccuracy.

(2) The code, based on the finite element partial differential equation solving package, TWODEPEP (IMSL, 1980) requires an initial distribution of nodes, or vertices, of the finite elements. If these nodes are not aligned with the contours of the source terms, they should be expected to migrate to where they are needed. Apparently, this is not happening, or if it is, something else is wrong in its functioning as evidenced by essentially random patterns in the alignment of the peaks of

the calculated concentration contours with the peaks of the source terms. Specifically, the peaks in the concentrations are showing up more or less around the origin (where the peak initial node density is located) or between it and the axial location of the source term peaks, but still hanging close to the origin.

(3) A set of strange systematics obtains when ratios are taken between the peak values obtained by this code and those obtained by DIFKIN. These systematics may hold the key to the inner working of TWODEPEP in relation to its implementation in DIFKT, and the problems which are being encountered in the functioning of DIFKT.

(4) The diffusion kinetic calculation being attempted with DIFKT for the deposition problem is for the full kinetic system of neutrals, ions and thermal electron. The species which show themselves to be most sensitive to the nonalignment of node distribution and source contours are the ionic species (see Figs. 7.1-2). Their concentrations show a strange but consistent asymmetry as a result. The vastly different time scale of these reactions from that of the neutrals (for the conditions being calculated) presumably plays a role. The global recombination approach devised here may alleviate this problem for DIFKT.

In results of runs of DIFKT at 100 eV, where the spatial grid was left the same as for 1 keV, as a result, the discretization of the source was crudified by about a factor of 10 (since at this low energy the short range term predominates over the long range, so the decrease

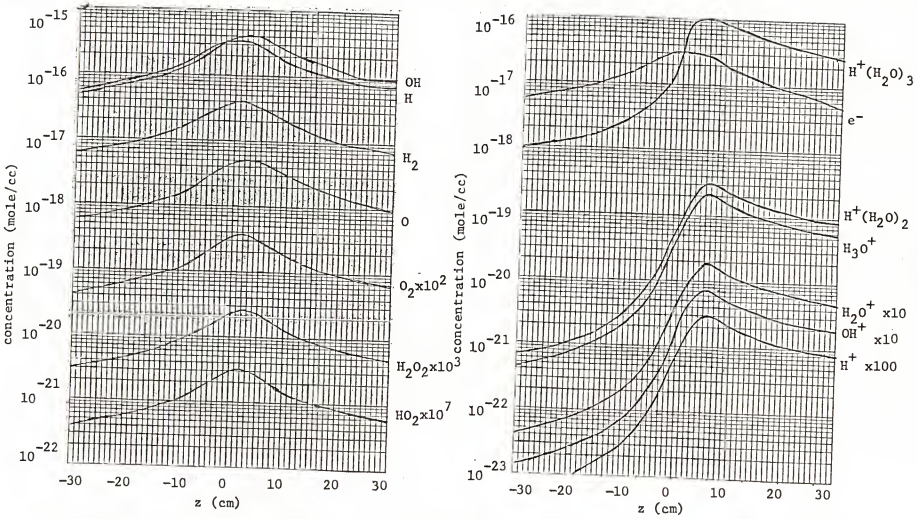

Figure 7.1. Results of DIFKT for the low density, slow chemistry case (unpublished work of Rio, Dayashankar, Schippnick, and Green) for (a) neutral species, and (b) ionic species and thermal electron.

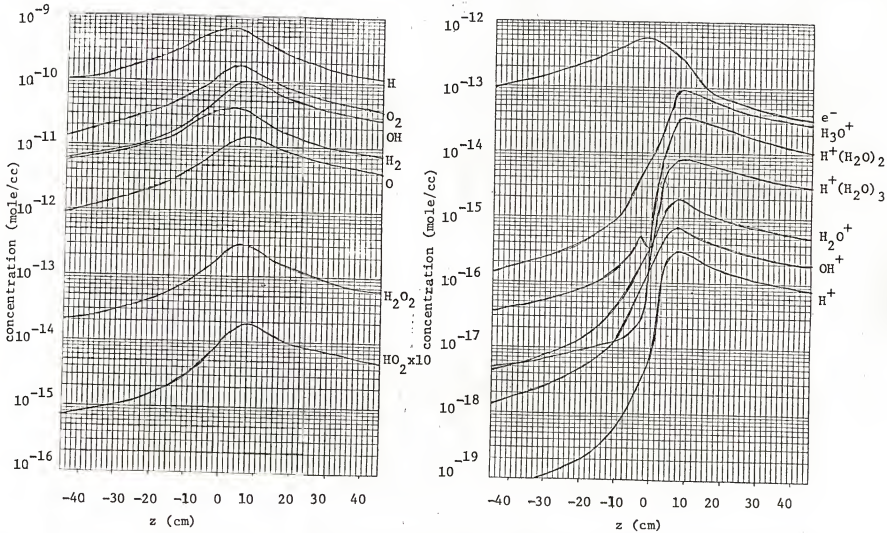

Figure 7.2. Results of DIFKT for the low density, borderline chemistry case, (unpublished work of Rio, Dayashankar, Schippnick, and Green) for (a) neutral species, and (b) ionic species and thermal electron.

in range is still more than what it would be if the E_o dependence of the long range were the only factor). As a result, in these runs the effect of the axis offset discrepancy with the location of the node distribution peak (the origin) was nil. In this case, the concentration contours of the ions did not show an asymmetry. In fact, they presented extremely narrower profiles in this case. This result is an interesting one, and may provide a further clue in our search for what is going wrong in the functioning of this code.

One aspect of the functioning of DIFKT which may play a role in the above problems is the mode of coupling it implements. As a result of the limitation of TWODEPEP to couple five separate variables at one time, the coupling between all concentrations is realized by coupling them in fixed groups of five per iteration; the coupling between groups is effected by the iteration step in the reassignment of values. The question naturally arises--what effect is there in grouping one way rather than another?

DIFKIN may be of use in the upgrading of DIFKT in the following way. DIFKT allows for initial estimates of the solution. Convenient analytic forms have already been established here for most of the forms which the steady state concentration profiles take. In this way, say, in application to particularly nonspherical spatial yield contours, the spherical approximation solution can be obtained via DIFKIN, modified to a nonspherical shape, and used as an initial estimate in DIFKT. It would be interesting to see what effect this would have on the rate of convergence of iteration, and on the level of accuracy of the final answer, in DIFKT.

In spite of the defects in the results obtained from DIFKT so far, they are in fairly reasonable agreement with the results of DIFKIN. Specifically, DIFKT has been run for the two low density cases presented in Chapter VI, very late chemistry and somewhat fast chemistry. These results (Rio, Dayashankar, Schippnick and Green, unpublished work) are displayed in Figs. 7.1-2. The results for the late chemistry case are in better than order of magnitude agreement with the results obtained here (Fig. 6.18). This is interesting in regard to the chemical product species, in regard to the distinction between near steady state and actual steady state. It is quite possible that the iterative procedure acts like a pseudotime (in a very distorted sense, but comparable). This idea was proposed by Rio (private communication, 1983).

The results for the fast chemistry case are also in better than order of magnitude agreement with the results obtained here (Fig. 6.19). Two points regarding the comparison here and in the previous case should be noted. First, the spatial yields inputs implemented in these steady state calculations are essentially spherical (axis ratio, .97). Thus, the two results can be compared straight across in this regard. (The worrisome axis offset here is 8.6 cm.) Second, DIFKT is calculating for the full ion-neutral-electron system. The results obtaining, if they be true results, should for that reason not be in complete agreement with the results obtaining from DIFKIN. The degree of this difference resulting from the global instantaneity approximation remains to be determined. In this regard it should be noted that the spatial yield inputs used in this calculation by DIFKT were not

corrected for any discrepancy in charge balance. This should be looked after in future work, as to the sensitivity of the calculation to this factor.

It is reassuring that the initial ion species appear at the lowest concentrations, reflecting the efficiency of reaction with H_2O. It is interesting that in both cases $H^+(H_2O)_3$ predominates over H_3O^+ and $H^+(H_2O)_2$. It is not clear how this relates to the fact that its reaction rate with the electron is the fastest of the three. It may relate to the fact that it is the last one to be produced, although in the pure kinetic case that fact correlates with it being the one in lowest ambient concentration. This is an open question since, for one thing, the overall accuracy of this calculation is uncertain.

We conclude that the code, DIFKT, has good promise, but still suffers from some nagging problems, which have yet to be resolved. With more work, these problems should be resolved. It is worth noting in this regard that the IMSL package, TWODEPEP, has been thoroughly tested and used by many users over the last 10 years or so, successfully and accurately (for example, see Mooney, 1984). Because DIFKT still gave assorted errors when tested with simpler systems, such as those considered in Chapter III, we are led to conclude that there are errors in the way in which it implements TWODEPEP.

Proposed Experimental Tests

Experimental identification of 'initial' spatial yields, i. e., spatial yields of various excited states created by the energetic degradation of the primary electron and its secondaries, etc. is

facilitated by the emission of characteristic wavelengths associated with these excited states when they decay to lower states and, finally, ground state. On the basis of line of sight detection of these emissions, the spatial distributions of the excited states which emit them may be inferred via Abel inversion (Cohn and Caledonia, 1970).

The earliest such work, and, to this day, definitive in its results, was the work of Grün (1956) for 5-54 keV electrons incident in air at 700 Torr. The later work of Cohn and Caledonia (1970) was for 2-5 keV electrons incident in N_2 at 0.69-2.8 Torr. In both cases spatial contours are shown very similar to the spatial contours of Monte Carlo generated spatial yield spectra presented in Fig. 2.10. Later work by Barrett and Hays (1975) obtained similar results.

In order to identify spatial distributions of chemical species (i. e., ground state species) in the diffusion kinetic evolution of the irradiated medium, a different approach is necessary. If the species of interest undergoes a transition lying in a detectable wavelength band, with linear absorption characteristics (i. e., obeying Beer's law) or at least known absorption characteristics, then its presence can be detected via absorption spectroscopy. Again line of sight detection can be utilized, and a variation of Abel inversion devised to infer spatial distribution.

In the case of electron bombardment of H_2O, the only species whose characteristic spectra lie in the optical or ultraviolet are OH (309.5 nm), H (Lyman α , 121.6 nm) and O and possibly HO_2.

In this connection, the pulsed radiolysis work of Hanrahan and coworkers (this campus, see for example Ramirez, Bera and Hanrahan, 1984) is of interest. A brief description of their work follows. A

Febetron electron beam generator (Bera and Hanrahan, 1984) is used which typically produces a 0.6 MeV beam of about 3 nanoseconds duration. The beam energy can be taken down to about 0.3 MeV but not much lower because of the parallel charge-series discharge arrangement of the capacitor bank used to generate the beam. The medium consists typically of about 600 Torr buffer Ar gas, variable amounts of water vapor (in the range 0.5-15 Torr), and reactive substrate. Concentration of OH is monitored over a 10 μsec interval. This measurement is not spatially resolved. Presumably, it is possible to do so.

Whether the possibility exists of carrying out continuous beam experiments which would correspond exactly to the configurations calculated for in this thesis is uncertain. It is a generally held opinion (Hanrahan, private communication, 1984) that continuous beam generators generally do not exist. Another consideration is the interrelationship between beam energy, medium density, spatial range, duration of pulse and desired duration of pulse. As density increases, the time of near steady state decreases (diffusion time). Spatial range also decreases. A minimum range is defined by maximum spatial resolution of detector. Most probably, a fast chemistry system which does not overheat (at least several atmospheres) would require too high a spatial resolution to be practicable. The load of the increased pressure on differential pumping of the electron gun (for example see Grün, 1956) also has limit and imposes one. That which it imposes is the convective disturbance near the gun. Thus a spatial range too small would be entirely engulfed in this. The condensation point limit of H_2O vapor pressure must also be taken into account.

The above discussion is meant only to be very preliminary. Experimental realization of continuous beam systems may be possible. However, the indications are that it is not. As an alternate route by which the radiological work carried out in this group may link up with experiment, the pulsed radiolysis work of Hanrahan and coworkers offers itself as a real possibility. Towards this end the following plan of work appears feasible: 1. Extend the spatial yield spectrum to higher (relativistic) energies. 2. Calculate the spatial yield spectrum for mixtures of gases, according to the prescription given in Singhal and Green (1982), which is based on the near universality of the spatial yield spectra for all gases. In this way, electron yield, Ar yield, and the initial yields of H_2O radiolysis are easily arrived at. 3. Modify DIFKIN to calculate in cylindrical geometry. 4. Run DIFKIN for an initial pulse rather than a continuous pulse beam. 5. Calculate pure diffusion results via Green's function integral for cylindrical geometry for initial pulse. 6. Calculate pure kinetic results for initial pulse, also over g-h grid, to enable isolation of diffusion effect in comparison of diffusion kinetic result with pure kinetic result.

Summary and Conclusion

The problem of diffusion kinetics for continuous, steady electron beam injection in water vapor has been addressed in a time dependent context. Certain approximations have been implemented in order to facilitate calculation. Quantitative limits of the ranges of applicability of these approximations, and quantitative estimates of the accuracy of these approximations have either been made, or the means

with which to do so have been produced. For example, in the case of the approximation of global instantaneity of charge recombination, it was observed that the effect of the approximation is limited to the H radical yield, as far as the neutral chemistry is concerned.

The other significant approximation which has been made is the sphericalization of the deposition contours. Referring to the steady state axisymmetric diffusion result calculated in Appendix C, and to the degree of eccentricity of the deposition contours, it is clear that little has been lost by this for contours which are not highly confocal.

It has been striven here to treat every aspect of the problem in as quantitative, rigorous and thorough a manner as possible. Where there have been uncertainties, such as in regards to the stiffness problem, or possible numerical artifacts of the radial grid, they have been pointed out.

Data display. Close attention has been paid to the display of data. For the sake of clarity and convenient visual display, several results have been presented in more than one format. The case of net production rates is particularly relevant because it is so difficult to estimate a slope from data, and because this result is at the heart of the stiffness problem. This result illustrates the importance of checking results.

In the preliminary work to this thesis, presented in Chapter II, display of data has also played an important role, and can be expected to play an even more important role in the continuation of this work in pursuit of an optimal analytic form by which maximal accuracy can be achieved in the analytic representation of the spatial yield spectra. What is envisioned, along with residual plots, are discrete bin band-

contour plots, where intervals are contoured, by which we can actually "see" the data. Without visual aids of this sort, identification of patterns and trends is severely hindered by the tediousness of manual plotting of a few representative cases.

Expense of the code. A point which has played a role of some importance in this work has been the expense of the code. Because the implicit linearized calculation of the chemistry in the BOAT code solves a system of n simultaneous linear equations at each grid point (where n is the number of species), the cost of the code is primarily a function of the number of species.

The size of the "chemistry friendly" time step also bears on the cost of the code, but less, because the major source of cost is in the logarithmic growth of time step at long times which is a result of the logarithmic evolution of the grid point distribution. This evolution is best kept logarithmic to insure that the grid point redistribution adequately cover the evolving steady state core. However, it can probably be made to move along faster without significant loss of accuracy. The advantage here can probably be enhanced by replacing Simpson rule interpolation by cubic interpolation. This would be beneficial for accuracy in general. It should also be possible to freeze out the core as it evolves. In this way a significant economization could be attained.

However, if the full system of ions, neutrals and thermal electron were to be calculated for, the expense due to "chemistry friendly" time step, as well as the expense due to the increase in the size of the system of simultaneous linear equations being solved for, would add up to a significant increase in expense.

Calculating on an IBM/370 type machine, one marching step requires 0.08 sec of cpu time for a 21 point grid for the full neutral system. The number of steps in the diffusion kinetic runs presented in Chapter III and Chapter VI gives an idea of the typical expense of this code. At the extreme of slow chemistry, the low density, 1 atm, and liquid runs took 19320, 17523, and 16574 steps, respectively. At the extreme of fast chemistry, the 1 atm and liquid runs took 30645 and 28788 steps, respectively.

Checking of code. The code has been checked out in detail, and found to give very accurate results when compared with known analytic test cases (Chapter III). These test cases include pure diffusion, checked against the Green's function calculation, pure kinetics for one and two species systems, steady state diffusion kinetics for single body decay, checked against analytic results, and steady state diffusion kinetics for one species two body decay, checked against analytic results in its asymptotic limits.

Approximations. Calculating for an incident energy of 1 keV, which was taken as a convenient representative value from which meaningful extrapolation both above and below is possible, provided a further convenience in that for the spatial yields at this incident energy, the short term component is negligible, and a single term exponential representation is possible. As a result, the analytic work pertaining to diffusion and diffusion kinetics, in which it was desired to use a source term of the same form as in the physical problem, was greatly simplified.

However, whether single or double, the exponential form is deficient in the following respect, namely that, the slope is not

continuous at the peak. It is easy to construct such a form. Two possibilities are (1) in general, the mapping, $e^{-\beta r} \rightarrow e^{-\beta f(r)}$ where $f'(0) = 0$ and $f(r) \sim r$ as $r \longrightarrow \infty$, and (2) the weighted difference of two exponentials, $(\alpha e^{-\beta r} - \beta e^{-\alpha r})/(\alpha-\beta)$. The latter enjoys the advantage of a linear sum in the pure diffusion result of its individual terms. However, once the nonlinear kinetic term enters in, it possesses no more of an advantage than the other.

Why this point can matter is that the 'reaction time' of the diffusion kinetic system has been defined in terms of the peak values of the spatial yields. We would therefore like to have the most accurate representation of the spatial yields that we can obtain. However, considering that the overestimation which comes as a result seems to be small, considering the profiles of spatial yield spectra and deposition spectra displayed in Chapter II, the overestimation introduced in reaction time is mitigated by the square root, we may conclude that this overestimation is fairly minor.

A very important step in the course of this work was the identification of the 'final' or post-recombination yields in terms of the 'initial' yields. It was at this point that we introduced the approximation of globally instantaneous charge recombination. Although this step allowed us to shrink the problem down to more manageable proportions, greatly economizing the computer code, as was noted above, it also washes out a very real effect, namely the effect of charge separation. It is therefore with very real interest that we look forward to the upgrading of this code in order to take charge separation into account.

Later, after identifying the dependence of ion reaction time scales on medium density and injection rate—by way of rather simple considerations, it became possible to quantitatively identify the dependence on medium density and injection rate of the separation of ion and neutral time scales or the lack of it. Specifically, they were found to merge for density near that of liquid and for injection rate at about the early/late chemistry boundary.

In this situation charge recombination can no longer be viewed as even locally instantaneous, and whether there is charge separation or not, it becomes necessary to accommodate noninstantaneous charge recombination via a split time step, which is what was envisaged in order to accommodate charge separation, anyway. The fix-up of the code is the same in either case. This result provides all the more impetus to upgrade DIFKIN in this way.

Physical relevance. Without physical relevance, the diffusion kinetics calculations become merely a mathematical exercise. In the interest of securing physical relevance, the heating rate by the electron beam of the medium has been estimated, albeit roughly, without taking into account energetics of the reactions, or the details of the energy loss process in the initial deposition.

Experimental verification. This is an appropriate point to next turn to experimental verification. Certain obstacles seem to be present here, even in the cases in which overheating does not appear to be a problem. These are, specifically—limits on the duration of a continuous pulse, limits of spatial resolution of spectroscopic detectors to, perhaps, the 0.1-1 mm range, possible wind effects at the tip of the electron gun due to differential pumping. In this connection

the technique of an aluminum window may be of use. It can also serve as a downstepper of incident energy in the CSDA limit where collimation and monochromaticity would not be much affected. Boundary effects on spatial yields in the backplume are, of course, unavoidable either way.

An alternate future plan of work has been proposed which may prove useful in collaboration with Hanrahan and coworkers. The feasibility of such a plan seems within the realm of possibility.

Extrapolation to liquid density. We may lastly mention one aspect of the work, the extrapolation to liquid density, which may be of some significance. In the first place these cases are physically realizable, since heating is not a problem for the injection rates considered. They have, however, two deficiencies. One is that they are calculated from spatial yields which are calculated on the basis of gaseous phase energy loss processes. Referring to the work of Kutcher and Green (1976a), we find that they were able to model the effect of the plasmon (the collective excitation mode in the liquid) on energy loss in liquid water by a broadening of the general oscillator strength peak in energy, and found a modest effect on W value. Referring to the later work of Turner et al. (1982), we find 25-30% differences reported in calculations of ratio of ionization cross section to total inelastic cross section (ionization plus excitation). A similar difference is seen in the peak of mass stopping power; however, slowing down spectra for 1 keV and 10 keV electrons are not seen to differ greatly over several orders of magnitude. One is led to the conclusion that such extrapolation of spatial yield may be of at least fair accuracy. This first deficiency is perhaps then not so great.

Secondly, the aqueous electron (Kupperman, 1974; Hanrahan, 1983) and aqueous OH^- and their reactions (Kupperman, 1974) have not been taken into account. This could be a more serious matter. However, it should not prove difficult to encode kinetics for a new set of species and reactions. We may then compare with results obtained using only gaseous phase reactions. Results presented here, based on the assumption of local instantaneity in the case of the kinetics, and global instantaneity in the case of the diffusion kinetics, have introduced still more approximation. As was pointed out above, the assumption even of local instantaneity in the case of liquid water is on the very borderline of validity. Given these differences, it would seem premature at this point to make any predictions concerning comparisons.

Conclusion

In conclusion, we may say that we have considered in rather thorough detail what would happen if a continuous, steady electron beam, suddenly turned on, were injected into a target of water vapor. The time scales, principal pathways, the effect of diffusion, the dependence on medium density, injection rate, temperature, and incident energy have all been considered in detail.

One thing which was not done, but which would have provided very valuable information, and should be done in future work, would have been to calculate and display reaction rates and reaction-specific production rates at r=0 in the diffusion kinetic case, for comparison with the corresponding pure kinetic rates. This information can still be extracted from the data stored on tape of the runs which were made, and should prove very interesting.

To the purpose of this thesis a computer code has been developed, which is capable of being upgraded, so that effects so far not considered may also be investigated, thereby extending the applicability of this work. The fact that this code was adapted from a vastly different code written for a vastly different purpose (and that, along the way, this original code had been adapted in a not so extreme way to a more similar problem) attests to the robustness of the numerical machinery, and the excellent utilitarian concept in the design of this original code.

Because the code is time dependent, it should prove equally capable of calculating for the associated problem of an initial pulse beam. This may be of more practical, immediate use in consideration of present experimental capabilities. Many of the mathematical tools developed and arrayed here, and a great deal of the methodology developed here, should prove useful in such a work.

APPENDIX A
ADAPTATION OF THE BOAT CODE

The BOAT code, written by Sanford Dash and Harold Pergament of Aeronautical Research Associates of Princeton Associates, Inc. for the U. S. Army (Dash and Pergament, 1978) to calculate turbulent jet entrainment with chemistry in rocket exhaust plumes, may seem like an unlikely place to start in order to base a code which should calculate diffusion kinetics, whether time dependent or steady state, for electron beam injection in a gas. However, this code does many things and can be adapted in many different directions. Finding a meeting place half way in between what this code can do and what one may want to apply it to can make a difference. In order to better appreciate this, the place to start is with a brief description of what the BOAT code is, what it does, and what options it provides.

In its most glorious form, the BOAT code consists of three job steps: PROCES, SCIPPY and BOAT. The first step reads in data and puts together a chemical system of species and reactions as directed, referencing its list of species and their thermodynamic data (for the purpose of calculating enthalpies, specific heats and Gibbs free energies--contained in the form of polynomial fits based on JANNAF Table data) and its list of reactions and reaction rate parameters.

The second step calculates supersonic aerodynamic inputs for the third step, if applicable, via what is known as an "overlaid" procedure, and can be bypassed. For our purposes then, it can be bypassed. The third step, which we are most interested in, calculates

turbulent jet entrainment (modelling by an effective diffusion) with chemistry in the flowfield of the exhaust plume. It can therefore be said to calculate steady state diffusion kinetics in an axial flow field.

The first point of arrival to which it was desired to take this code was to apply it to the problem of axisymmetric laminar flames, both diffusion and pre-mixed (see Kanury, 1975).

The next requirement was to debug the code of a few lingering errors and typos, of which two had to do with the encoding of two of the five reaction type pairs which are encoded in BOAT:

(1) $A + B \rightarrow C + D$

(2) $A + B + M \rightarrow C + M$

(3) $A + B \rightarrow C + D + E$

(4) $A + B \rightarrow C$

(5) $A + M \rightarrow C + D + M$

where (6) - (10) are the corresponding two-way reactions. These four reaction types (3,8; 5,10) are not represented in the six standard chemical systems built into the code, which leads me to believe that they had never been checked.

The next and final step was to adapt the code to this particular problem. The numerical machinery of the BOAT code (job step three) accomplishes the following. The hydrodynamic equations of axial flow combined with radial diffusion in streamline coordinates govern the conservation of angular momentum, energy or enthalpy, and species. If nonlaminar viscosity is opted for, then equations governing conservation of turbulent kinetic energy and turbulent dissipation are also

included. However, in the laminar mode these equations are not included. The three equations of interest, as they appear in BOAT, are

$$\frac{\partial u}{\partial x} = -\frac{1}{\rho u}\frac{dp}{dx} + \frac{1}{\psi}\frac{\partial}{\partial \psi}\left(A\frac{\partial u}{\partial \psi}\right) + \frac{\rho_e - \rho}{\rho u} g \tag{A.1}$$

$$c_p \frac{\partial T}{\partial x} = \frac{1}{\rho}\frac{dp}{dx} - \frac{1}{\rho u}\sum_i h_i \dot{w}_i + \frac{1}{\psi}\frac{\partial}{\partial \psi}\left(\frac{c_p}{Pr} A\frac{\partial T}{\partial \psi}\right)$$

$$+ \frac{A}{\psi}\left[Z + \frac{Le}{Pr}\sum_i c_{p_i}\frac{\partial F_i}{\partial \psi}\right] \tag{A.2}$$

$$\frac{\partial F_i}{\partial x} = \frac{1}{\psi}\frac{\partial}{\partial \psi}\left(\frac{Le}{Pr} A \frac{\partial F_i}{\partial \psi}\right) + \frac{\dot{w}_i}{\rho u} \tag{A.3}$$

where u is axial velocity, v is radial velocity, x is axial coordinate, ψ is streamline coordinate or streamline function, T is temperature, μ is coefficient of viscosity, ρ is density, ρ_e is ambient edge density, and g is acceleration due to gravity, c_p is specific heat, $F_i = X_i/W$ where X_i is mole fraction of i-th species and W is mixture molecular weight, p is pressure, h_i is enthalpy of i-th species, r is cylindrical radial coordinate, $\dot{w}_i$ is net rate of production of the i-th species, and Le is Lewis number and Pr is Prandtl number (see Kanury, 1975), and the quantity A is given by

$$A = \mu \frac{\rho u r^2}{\psi} . \tag{A.4}$$

The tranformation from (x,r) to (x,ψ) is given by

$$\psi \frac{\partial \psi}{\partial r} = \rho u r \tag{A.5}$$

$$\psi \frac{\partial \psi}{\partial x} = -\rho v r \tag{A.6}$$

In the case of constant pressure mixing the pressure gradient term in the axial momentum and energy equations drops out.

The mystery term Z is stated by the authors to be $(\partial u/\partial \psi)^2$, but its stated discretization corresponds to $\partial^2 u/\partial \psi^2$. It is encoded as u^2. By comparison with other standard treatments (for example, see Miller and Kee, 1977) it is apparent that this term represents a small correction to "stagnation" enthalpy and can be neglected at lower velocities.

This set of equations is parabolic in the axial coordinate, and therefore a parabolic marching technique is implemented to solve it for given nozzle conditions ('initial' conditions) and given mixing layer boundary conditions, i.e. at the edge which moves outward radially with increasing x. The radial coordinate is transformed via the von Mises transformation to the streamline coordinate, ψ, and the streamlines are evolved, via enthalpy conservation, so that the radial grid is made to follow along constant streamlines, equally spaced in streamline function, ψ. The streamline evolution is accomplished via grid-point redistribution technique which incorporates a cubic interpolation rule. This grid-point redistribution technique is one of the state of the art aspects of the code. However, its usefulness is limited to the flowfield expansion context.

We may note in passing that as a result of transformation to streamline coordinates, the equation of continuity,

$$\frac{\partial \rho u}{\partial x} + \frac{1}{r}\frac{\partial}{\partial r}(\rho r v) = 0 \tag{A.7}$$

is solved for automatically.

The contribution of the mass flux term in the energy equation is taken into account via a predictor-corrector method in enthalpy, inverting temperature from enthalpy at each step, based on the previous value.

The kinetic production-destruction terms are calculated via an implicit linearized approach. This technique is known to guarantee numerical stability. The implicit linearization is given by

$$(F_iF_j)_{n+1} = (F_iF_j)_n + F_{jn}[(F_i)_{n+1} - (F_i)_n] + F_{in}[(F_j)_{n+1} - (F_j)_n]$$

$$= -(F_iF_j)_n + (F_j)_n(F_i)_{n+1} + (F_i)_n(F_j)_{n+1} \tag{A.8}$$

$$(F_iF_jF_k)_{n+1} = -2(F_iF_jF_k)_n + (F_jF_k)_n(F_i)_{n+1}$$

$$+ (F_iF_k)_n(F_j)_{n+1} + (F_iF_j)_n(F_k)_{n+1} \tag{A.9}$$

Here the subscripts indicate axial station. Since the values at station n are known, the values at station n + 1 are to be solved for. They are therefore said to be defined implicitly. They are obtained by solution of the simultaneous system of linear equations which the linearization technique implies.

Application to Laminar Flames

The adaptation of the BOAT code to the laminar flame problem required the following modification of the BOAT code numerical machinery. In place of constant values of Lewis and Prandtl numbers, temperature dependent values were required. The values implemented in the BOAT code for these dimensionless numbers were constants of order unity. Since they are temperature dependent and inside the streamline derivative, the finite spatial differences had to be rewritten to include their spatial variation (as a result of nonzero temperature gradient).

Noting the standard definitions of these dimensionless numbers (Kanury, 1975), it becomes clear that the ratio, Le/Pr, appearing in the mass flux term in equations (A.2) and (A.3) is incorrect, and should be replaced by 1/PrLe. It is worth going over the details. The standard definitions, taken from Kanury (1975), are

$$Pr \equiv \nu/\alpha = (\mu/\rho)/(\lambda/c_p) \tag{A.10}$$

$$Le \equiv \alpha/D = (\lambda/c_p)/D \tag{A.11}$$

The viscosity factor, $A = \mu\rho ur^2/\psi = \nu\rho^2 ur^2/\psi$, and the thermal factor, $c_p A/Pr = \lambda\rho ur^2/\psi$, are correct as they stand. The correct mass flux or diffusion factor is $A/PrLe = D\rho^2 ur^2/\psi$, not LeA/Pr.

Finally, it should be noted that in the laminar flame application constant pressure mixing is assumed, as a result of which the pressure gradient terms in Eqs. (A.1) and (A.2) drop out.

This modified BOAT code was implemented to solve for various flame conditions: both H_2-air and CH_4-air, both diffusion and pre-mixed. Interesting results were obtained, especially in comparison with published results of Miller and Kee (1977), Kee and Miller (1978), and with our own experimental data (Pamidimukkala et al., 1983). However, the author's involvement on this project was terminated for lack of funds. Fortunately he could be supported by the radiological grant by applying this code to the radiological problem.

Application to the Radiological Problem

The following problem is now posed. Adapt the BOAT code to the problem of diffusion kinetics for an electron beam incident in water vapor. This problem is parabolic in time coordinate, and elliptical in spatial coordinate. The BOAT code, which in effect, calculates steady state diffusion kinetics in an axial flowfield, solves a parabolic problem in two dimensions.

The general radiological problem, being axisymmetric, involves one parabolic dimension, time, and two elliptical dimensions, namely, the two spatial coordinates, say, cylindrical coordinates.

One logical choice therefore greets us: either pose the radiological problem in one (radial) spatial coordinate, or expand the BOAT code to cover a two dimensional half-azimuthal grid. The decision was made to go the first route.

The idea occurred of constructing a generalized orthogonal coordinate system of radial type, ellipsoidal in shape, in order to allow calculation in a somewhat more faithful spatial form. The

author's idea was that if the contours were made to be spherically asymptotic, therefore realistically reflecting the trend of diffusion, in fact, the trend of the initial radiological deposition process as well, that by neglecting tangential diffusion a one dimensional approximation to two-dimensional diffusion would be possible.

Such contours were actually encoded, and this work is described in Appendix B. However, two things happened: (1) an esoteric impasse developed in the checking out of the coordinate system. Calculated pure diffusion approach to steady state showed tolerable drift at the origin for the polar coordinate ranging from the radial direction to infinitesimally close to the axial direction ($\eta = 0.999999$). However, in going over to polar contour along the axis ($\eta = 1$), a jump occurred which the author could not explain (see Fig. A.1). (2) Typical deposition contours at incident energies up to and around 1 keV proved to be of sufficiently low eccentricity so that a spherical approximation would suffice.

It was then decided to go ahead with this work in the spherical approximation. It should be noted in passing that it should also be easy to adapt the code to the case of cylindrical geometry. As to the general case, it would seem that after the esoteric impasse is overcome, the generalized radial coordinate system could prove useful in the implementation of a two dimensional grid. The advantage that it could provide would be the following. With contours aligned with the source in the core region and asymptotically spherical in the limb, an optimal representation would be provided at minimal expense, i. e. with a minimal polar grid.

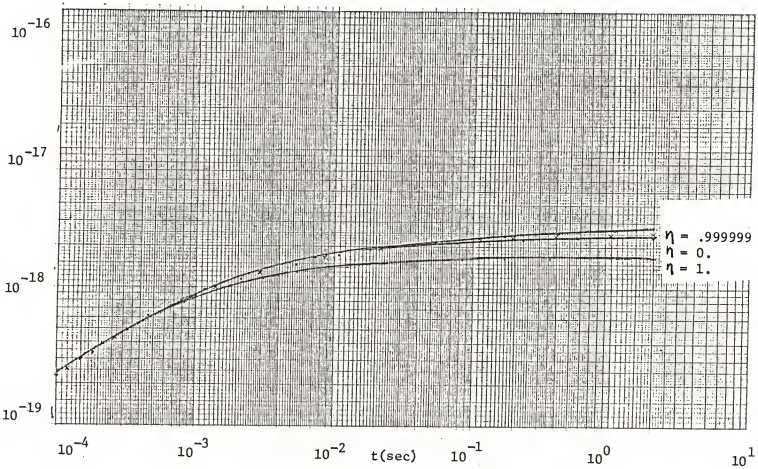

Figure A.1. Pure diffusion time course at $\xi = 0$ for $\eta = 0$, .999999, and 1. Results of numerical code implementing one dimensional approximation.

Subroutine Organization of DIFKIN

In this section the subroutine structure and function of DIFKIN are summarized in order to provide a user's guide to the code and to document the adaptation from BOAT. With the first aim uppermost in the author's mind, the summaries here have been made as complete and as clear as possible.

Job Step 1:

1. MAIN -- reads in input data: chemical system index numbers, physical input data, control parameters (pointers and quantifiers), then writes the chemical system along with regurgitation of other inputs to temporary disk file which is read by subroutine SA in job step 2. Calls SYSMOD (optionally including entry point RRMOD) and DABANK (including entry points LOCOB and REACT).
2. SYSMOD -- constructs chemical system (references BLOCK DATA. entry point RRMOD rescales chosen reaction rates.
3. DABANK -- reads in species ID's, mol. wts., enthalpies of formation, and fitting parameters for thermodynamic functions from card image file "CHEMRAD" (named by author). It then reads in reactions, i. e. species entries, reaction type, and reaction rate coefficient parameters.

Job Step 2:

1. MAIN -- "home": 1. calls SA which reads in data from temporary disk file written to by MAIN (job step 1), 2. calls PREP (taken bodily from Rio's code DIFKT (Rio, Ph. D. thesis, 1983)) which reads in input data for calculation of spatial yields, namely plume integrals and spatial yield spectra parameters, input 3.

loops over. 4. calls SB, the initialization subroutine. (SB initializes the grid, the concentrations, and the yields), 5. loops on M1, the marching step driver, until it is flagged. It then calls O1 (entry point in OT), which writes permanent restart disk file, and then goes on to next point, if the last, then stops.

2. SL -- system of simultaneous linear equations solver. Gauss-Jordan pivot.
3. IC -- assigns initial conditions: value of 1. for H_2O, value of 10 for all others (concentrations in units of the H_2O concentration, mole fractions if dilute regime).
4. PREP -- described in MAIN.
5. YI -- extracted from Rio's code, DIFKT. Calculates spatial species yields via branching ratios over state yields, folded into spatial plumes of spatial yield spectrum (see Eq. 2.25). Post-recombination reassignment of spatial species yields is then made (this thesis, see Eqs. 4.3a-g, 4.5 and 4.6).
6. NR -- "Newton-Raphson, Euler". Calculates ξ-grid. Depends on value of η.
7. SIMSON -- Simpson rule interpolation. Two versions: previous dangerous version with convoluted search logic, later safer version with bubble search.
8. CC -- calculates entries in column vector and matrix implied by linearization of kinetic production-destruction terms. The encoding of this subroutine is extremely compact. This is

advantageous to computer efficiency but renders its content totally opaque to the user until after several hours of combinatorial and algebraic deciphering.

9. GX — calculates Gibbs free energy for each species.

10. EF — (function subprogram). Calculates Arrhenius factor for backward reaction rate if two way reaction type is opted. calls GX.

11. S2 — a. calculates forward (if one way) or forward and backward (if two way) kinetic production and destruction terms, then calls EF if two way, then calls CC which uses the above terms as inputs (see above); b. before returning, calls.

12. S3 — integrator engine: calculates finite difference diffusion Laplacian and implicit chemistry via call to SL using inputs from CC. Evolves all points except edge point. Center point (i.e., origin) is evoled separately via third difference extrapolation.

13. M1 — marching step driver: 1. calculates time step: only diffusion unless chemistry override is specified. if that is, then takes minimum of the two until diffusion time steps crosses plateau value of chemistry time step, after which for the sake of economy it takes the geometric average (calls function subprogram CHEM to evaluate chemistry time step); if pure kinetic run time step equals chemistry time step, 2. decides whether to print out results at this time station or not on basis of either (a) discrete blocks, 'unlimited' number (choice in original BOAT code was binary), or (b) newly coded exponential rate: $\Delta t_{pr} = c_{pr} t$, 3. calls IN to output updated

geometry of the grid, regurgitate miscellaneous physical input data, and output the spatial yields at the present grid points (if pure kinetic run, skip all this after first time station), 4. edge point extrapolation (second difference in logarithm), 5. calls M2, and 6. checks for final time exceeded, if so returns to loop in MAIN.

14. CHEM -- (function subprogram): calculates "chemistry friendly" times step. See (Eq. 5.1).

15. M2 -- two functions: 1. check for negative "mole fractions" (precisely, below -10^{-10}). if so, halve the time step and try again. if time step falls below minimum, print warning and stop. if "mole fraction" exceeds -10^{-10} but is exceeded by 10^{-65}, truncate to 10^{-65} and carry on, 2. grid point redistribution: evolve ξ_o, redistribute grid in discrete steps depending on whether or not

$$\frac{\text{new } \xi_o(t)}{\text{value at last print out}} > c_{int}$$

then call SIMSON to interpolate in the logarithm of the concentration over the transformed coordinate, $\zeta = \ln(\xi/\xi_o + 1)$.

16. IN -- writes out header and inputs. Adapted to write out updated geometric information, misc. physical inputs, and yields at updated grid points when called from M1 (see M1).

17. SA -- 1. reads inputs from temporary disk file written by MAIN in job step 1, 2. reads in diffusion coefficients at 300 K and 1 atm from unit 5, calculates diffusion coefficients at specified

temperature and density, 3. assigns numerical indices to each reaction to indicate species and positions (this aspect of original BOAT code required some debugging).

18. SB — initializes (1) ξ_o, (2) Gibbs free energies, (3) certain control parameters which change value through cycles, (4) initializes grid (calls NR), concentrations (calls IC) and yields (calls YI), and (5) converts (overwrites) initial "mole fractions" (molar concentration/molar concentration of H_2O) to "working units" (adapted term of Dash and Pergament), namely, "mole fraction"/mol.wt. of H_2O. "Working units" in original code were true mole fractions/mixing mol. wt.,

19. OT — 'output' — writes out concentrations as such or scaled by H_2O concentration [and other information to printer and to disk file]. entry point O1: writes out RESTART file (disk), entry point O2 (called from S2 if opted for): write out reaction rates.

Grid Point Redistribution and Time Step

The grid point redistribution scheme existing in the BOAT code was found to be inappropriate to our purposes. A new one was therefore written. Although a cubic scheme is preferable to handle inflections, if a transformed variable can be found in which the concentrations are inflection free or very close to it, then a Simpson rule is sufficient. A Simpson rule interpolating subroutine was written.

The distribution of the radial coordinate (ξ) grid is our next consideration. In the interest of optimal bin averaging we require that

the packing of the grid reflect the evolving concentration profiles. In order to accomplish this we set up an equally spaced grid in a transformed coordinate, $\xi = \ln(\xi/\xi_o(t) + 1)$ where $\xi_o(t)$ is a monotonic increasing function of t through ln t, chosen empirically, the purpose of which is to control the evolution in time of the grid redistribution, and through it, the time dependence of the time step (see Eq. A.1). As far as only the diffusion is concerned, the trade-off involved here is between cost and the accuracy of discrete covering of the central core. Accuracy in this is not critical to the overall accuracy of the calculation, and may be compromised to some extent, with negligible impact upon overall accuracy.

The grid endpoints in ξ are fixed at 0 and an edge point, $\xi_e = 36/\beta d$ (where d is medium density). The evolution at the edge point is accomplished through second difference extrapolation in the logarithm. The value $\xi_e = 36/\beta d$ is chosen since at this point the steady state diffusion profile has fallen off to 5% of its peak value at the center, for $y(r) = e^{-\beta dr}$.

The discretization of the Laplacian at the origin is accomplished through a third difference extrapolation and half-bin assignment (in order not to divide by zero).

Discretization of the derivatives with respect to ξ is accomplished through transformation of the derivatives with respect to the equally spaced coordinate, ζ:

$$\frac{\partial u}{\partial \xi} = \frac{d\zeta}{d\xi}\frac{\partial u}{\partial \zeta} \tag{A.10}$$

$$\frac{\partial^2 u}{\partial \xi^2} = \frac{d\zeta}{d\xi}\left[\frac{d}{d\zeta}\left(\frac{d\zeta}{d\xi}\right)\frac{\partial u}{\partial \zeta} + \left(\frac{d\zeta}{d\xi}\right)\frac{\partial^2 u}{\partial \zeta^2}\right] \tag{A.11}$$

Since

$$\frac{d}{d\xi}\left(\frac{d\zeta}{d\xi}\right) = -\frac{d\zeta}{d\xi} = -\frac{1}{\xi + \xi_o} \tag{A.12}$$

for the transformation, $\zeta = \ln(\xi/\xi_o + 1)$, the transformation formula for the second derivative is given by

$$\frac{\partial^2 u}{\partial \xi^2} = \frac{1}{(\xi + \xi_o)^2}\left[\frac{\partial^2 u}{\partial \zeta^2} - \frac{\partial u}{\partial \zeta}\right] \tag{A.13}$$

wherefore the interpolated second difference, $\Delta^2 u_i$ is given by

$$\Delta^2 u_i = \frac{1}{(\xi_i + \xi_o)^2}\left[(1 - \frac{\Delta\zeta}{2})u_{i+1} - 2u_i + (1 + \frac{\Delta\zeta}{2})u_{i-1}\right]. \tag{A.14}$$

The step size determination already existing in the BOAT code embodies the standard stability criterion (see Kupperman and Belford, 1961a),

$$\Delta t = \frac{1}{3}(h_1 \Delta\xi)^2_{min}/D_{max} \tag{A.15}$$

expressing diffusion control, with repeated halving of this value if negative concentrations result. The generalized difference $h_1 \Delta\xi$ (explained in Appendix B) reduces to Δr in the spherical case.

A "chemistry friendly" override time step has been added to accommodate the chemistry for pure kinetic runs and diffusion kinetic runs in the early or borderline chemistry regime.

In kinetic codes based on the Gear method (Hindmarsh, 1974), the time step is determined on the basis of the derivatives of the

solution. We find that a simple, empirical approach proves adequate in the context of the calculation of kinetic production - destruction terms via implicit linearization (Eqns. (A.8) and (A.9)) employed in the BOAT code. Specifically we find that the concentration time courses became stabilized (i.e. converged in function space) for $\Delta t(t)$ everywhere less than or equal to

$$\Delta t_{stbl} = \begin{cases} 0.1t, & t < \tau_c \\ 0.1\tau_c, & t > \tau_c \end{cases} \tag{A.16}$$

where τ_c is reaction time (see Chapter III, section 2). It was also found that this requirement could be relaxed somewhat for $t \gg \tau_c$ with slow logarithmic growth. This was very advantageous for economy in the context of the full diffusion kinetic calculations. These results are illustrated in the selection of kinetic time plots presented in Fig. A.2.

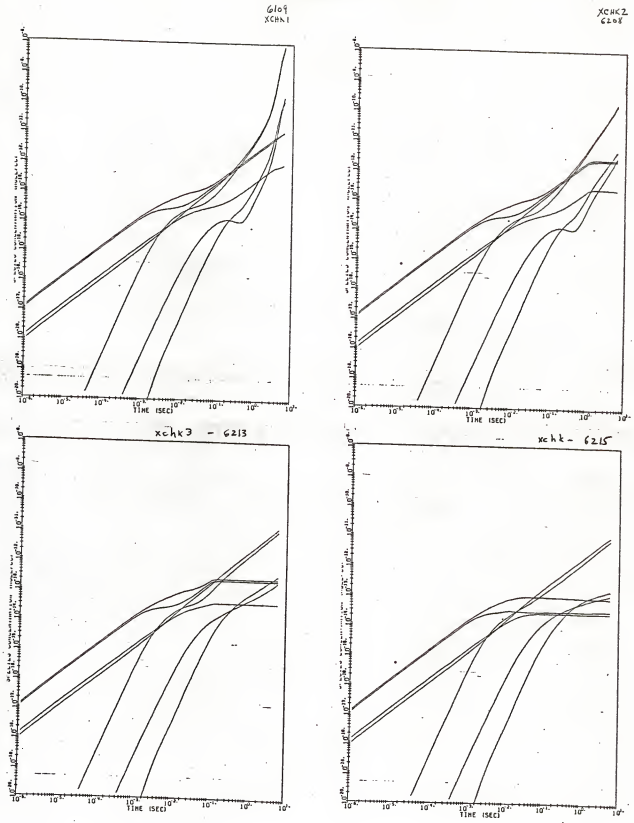

Figure A.2. Kinetic time courses for various choices of $\Delta t(t)$.

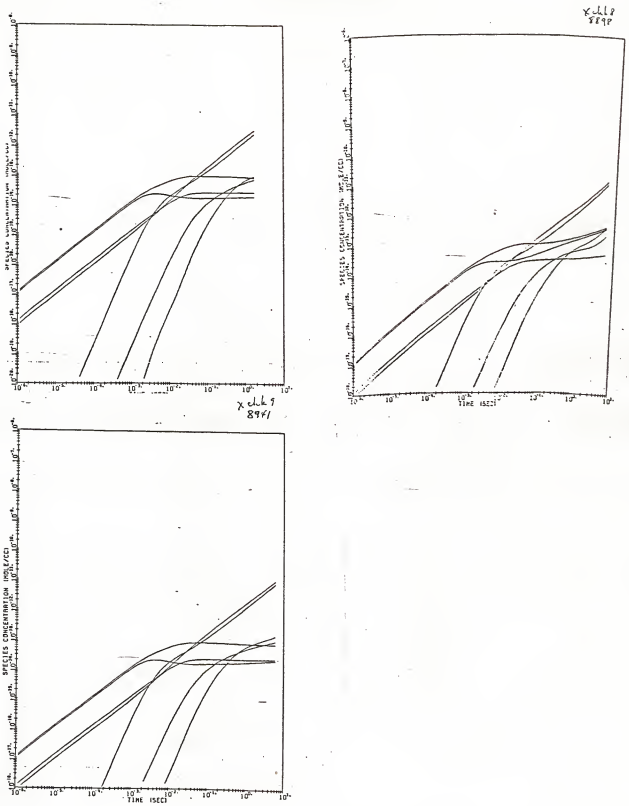

Figure A.2. continued.

APPENDIX B

GENERALIZED ORTHOGONAL COORDINATE SYSTEM OF RADIAL TYPE

An attempt was made to encode a generalized radial grid, and in fact came within a very small fraction of success. However, it became apparent that, aside from an esoteric problem that arose (see discussion in Appendix A), such a way to go would only really pay off if it were carried all the way to a two dimensional grid. Where it was left at was not very far from there. For the sake of documentation and reference, this work is presented here.

Let the orthogonal coordinates be ξ and η, where ξ is the generalized radial coordinate and η is the generalized polar coordinate.

We first choose to consider the case of the isocontours being concentric prolate ellipses:

$$\xi = \sqrt{\rho^2 + (z - z_o)^2/b^2(\xi)} \ . \tag{B.1}$$

The axis ratio parameter $b(\xi)$ is chosen to be a smooth, slowly varying function, monotonically decreasing from a maximum, not necessarily a stationary maximum, at $\xi = 0$ as $\xi \to \infty$. Referring to Appendix C where steady state axisymmetric diffusion is calculated, a lesson is gained concerning the limits of "intuition": the maximum of $b(\xi)$ at $\xi = 0$ for the steady state solution for source term of the form

$$y(\rho,z) = Ae^{-\sqrt{\rho^2 + (z-z_o)^2/b_o^2}}$$

(where b_o is a constant) is not stationary.

It may be noted that if ξ is thought of as a function of ρ and z, it may also be thought of as a functional of b. We may therefore write $\xi = \xi[b](\rho,z)$.

The perpendicular slope follows at once from Eq. (B.1):

$$\left(\frac{\partial\rho}{\partial z}\right)_\xi = \frac{b^2(\xi)\rho}{|z-z_o|} \; . \tag{B.2}$$

We now introduce the adiabatic approximation, where we consider $b(\xi)$ to be locally constant. Equation (B.2) then locally integrates to

$$k(\xi,\eta) = |z - z_o|^{b^2(\xi)}/\rho \; . \tag{B.3}$$

We now introduce the local coordinate, $\tilde{\eta}(\xi,\eta)$ which may be taken as any suitable monotonic extended analytic function of k. In order to regain the conventional definition in the spherical limit, $\eta = \cos\theta$, we set $\tilde{\eta} = k/\sqrt{1 + k^2}$ for $\rho > 0$, and $\tilde{\eta} = \pm 1$ for $\rho = 0$, $z \neq 0$. We now define the global or governing orthogonal coordinate, η, for the sake of definiteness, by the boundary condition, $\tilde{\eta}(0,\eta) = \eta$. (The other suitable definition would be $\tilde{\eta}(\infty,\eta) = \eta$.) It can be shown that $|\tilde{\eta}|$ is monotonically decreasing in ξ, with maximum $|\tilde{\eta}|_{max} = |\tilde{\eta}(0,\eta)|$ and minimum $|\tilde{\eta}|_{min} = |\tilde{\eta}(\infty,\eta)|$ for $0 < |\eta| < 1$, and stationary at the turning points, $|\eta| = 1, 0$. We may now construct the η-contours. This is done by integrating the first order normal differential equation given by Eq. (B.2) where the dependence of the right hand side on ρ and

z is implicitly defined with the help of Eq. (B.1). This is easily done numerically by the Euler method, by which we arrive at a span for ρ and ξ over an interpolatory grid in z for a given value of η. Contours of ξ and η are shown for $b(\xi)$ given by

$$b(\xi) = 1 + \delta\, e^{-\xi/\xi_b} \tag{B.4}$$

where $\delta = 0.6$ and $\xi_b = 7.4$ in Fig. B.1 where it is also used to display approximate characterization of the steady state solution for pure diffusion for source term with $b \equiv 2$.

The Laplacian operator in this generalized coordinate system, following Morse and Feshbach (1953), is given by

$$\nabla^2 u = \frac{1}{h_1 h_2 \rho} \frac{\partial}{\partial \xi} \left(\frac{h_2 \rho}{h_1} \frac{\partial u}{\partial \xi} \right) + \frac{1}{h_1 h_2 \rho} \frac{\partial}{\partial \tilde{\eta}} \left(\frac{h_1 \rho}{h_2} \frac{\partial u}{\partial \tilde{\eta}} \right) \tag{B.5}$$

where h_1 and h_2 are the scale factors of ξ and $\tilde{\eta}$. Following Morse and Feshbach, we note that they are given by

$$h_1 = \sqrt{\left(\frac{\partial \rho}{\partial \xi}\right)^2 + \left(\frac{\partial z}{\partial \xi}\right)^2} \qquad h_2 = \sqrt{\left(\frac{\partial \rho}{\partial \tilde{\eta}}\right)^2 + \left(\frac{\partial z}{\partial \tilde{\eta}}\right)^2} \tag{B.6}$$

The adiabatic approximation is invoked in the evaluation of the partial derivatives by implicit differentiation of Eqs. (B.1) and (B.3):

$$\partial \rho / \partial \xi = \xi \rho / \xi^2 [b^2] \qquad \partial z / \partial \xi = \xi (z - z_o) / \xi^2 [b^2] \tag{B.7-8}$$

$$\partial \rho / \partial \tilde{\eta} = - \frac{|z - z_o|^{2-b^2} s^3}{b^4 \xi^2 [b^2]} \qquad \partial z / \partial \tilde{\eta} = \frac{\rho^3 |z - z_o|^{1-b^2} s^3}{b^2 \xi^2 [b^2]} \tag{B.9-10}$$

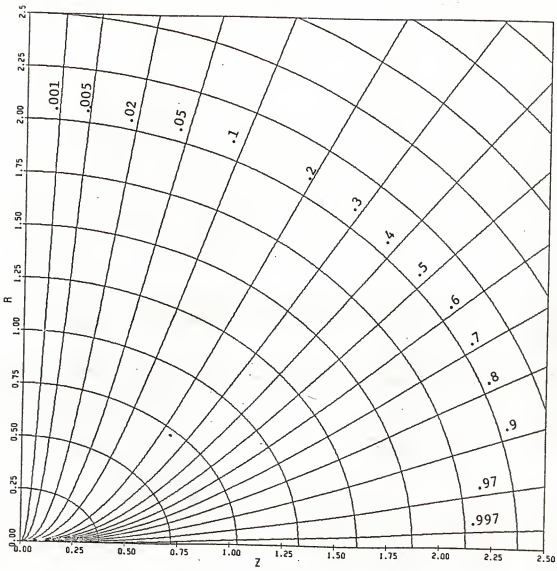

Figure B.1. ξ and η contours for $b(\xi)$ given in Eq. B.4 with $\delta = 0.6$ and $\xi_b = 7.4$, ξ contours are isocontours of approximate solution to steady state diffusion equation for $b_o = 2$ in source term given by Eq. C.9.

where $b = b(\xi)$, and, observing that $\tilde{\eta}/\sqrt{1 - \tilde{\eta}^2} = k(\xi,\eta)$, it follows that $s \equiv dk/d\tilde{\eta} = (k/\tilde{\eta})^3 = (|z - z_o|^{b^2}/\rho\tilde{\eta})^3$. It follows that $h_1 = \xi/\xi[b^2]$ and $h_2 = |z - z_o|^{1-b^2}\rho^2 s^3/b^2\xi[b^2]$.

In order to encode Eq. (B.4) the special cases $\xi = 0$ and $|\eta| = 1$ or 0 for $\xi > 0$ must be considered separately because of L'Hopital limits. The limiting form of the Laplacian is

$$\nabla^2 u = a_1 \frac{\partial^2 u}{\partial \xi^2} + \frac{a_2}{\xi}\frac{\partial u}{\partial \xi} \tag{B.11}$$

(in the ξ term) where $a_1 = 1$ and $a_2 = 1 + 1/b^2$ for $\eta = 0$, and $a_1 = 1/b^2$ and $a_2 = 2$ for $|\eta| = 1$, $\xi > 0$ and for $\eta \neq 0$, $\xi = 0$.

The sense of the values of a_1 and a_2 is made clear by considering the extreme possible limiting cases of the geometry of the problem: $b \to 0$ and $b \to \infty$. In the limit $b \to 0$ the metric becomes locally flat in the axial direction in the neighborhood of the axis, and therefore, a_1 must equal $1/b^2$ for scaling and dominate a_2 for $|\eta| = 1$. In the limit $b \to \infty$ the metric becomes locally cylindrical in the neighborhood of the z=0 plane, and therefore in this limit $a_1 = a_2 = 1$ for $\eta = 0$. In the case $b = 1$ the spherical metric is regained.

APPENDIX C
AXISYMMETRIC DIFFUSION--STEADY STATE

In order to justify spherical approximation it is useful to calculate pure diffusion in the general axisymmetric case. In the general axisymmetric case

$$R = \sqrt{r^2 - 2rr_o\left[\mu\mu_o + \sqrt{(1-\mu^2)(1-\mu_o^2)}\cos\phi_o\right] + r_o^2} \tag{C.1}$$

where $\mu = \cos\theta$ and $\mu_o = \cos\theta_o$, the Green's function integral (Eq. 3.24) is analytic in ϕ_o, and reduces to

$$c(r,\theta,t) = 2\pi\int_0^t \frac{dt_o}{(2\sqrt{\pi D\tau})^3}\int_{-1}^{1}\int_0^{\infty} y(r_o,\theta_o,t_o)r_o^2 dr_o d\mu_o$$
$$\times\, e^{-(r^2-2rr_o\cos(\theta-\theta_o) + r_o^2)/4D\tau}(1 + F(p)) \tag{C.2}$$

where $F(p) = e^{-p}I_o(p) - 1$ and

$$p = (2rr_o/4D\tau)\sqrt{(1-\mu^2)(1-\mu_o^2)}.$$

$I_o(p)$ is the spherical Bessel function of order 0. The time dependent problem reduces to a triple integral in r_o, μ_o and t_o. Although numerical calculation of the contribution to this integral in the region t_o not too close to t is straightforward, it becomes tricky in the region too close to t because the singularity of the Green's function in τ.

Rather than follow this out, we turned to the steady state solution, which is more easily evaluated, and provides suitable information about the broadening effect of diffusion on the deposition contours laid down by the source.

Expressing the diffusion Laplacian in spherical coordinates, the diffusion equation becomes

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c}{\partial r}\right) + \frac{1}{r^2}\frac{\partial}{\partial \mu}\left((1-\mu^2)\frac{\partial c}{\partial \mu}\right) + \frac{y(r,\mu)}{D} = 0 \qquad \text{(C.3)}$$

Expanding in Legendre polynomials in μ (Jackson, 1967), we set $c = c(r,\mu) = \sum_{\ell=0}^{\infty} c_\ell(r)P_\ell(\mu)$ and $y = y(r,\mu) = \sum_{\ell=0}^{\infty} y_\ell(r)P_\ell(\mu)$ where $y_\ell(r)$ is given by

$$y_\ell(r) = \frac{2\ell+1}{2}\int_{-1}^{1} y(r,\mu')P_\ell(\mu')d\mu'. \qquad \text{(C.4)}$$

Noting the identity

$$\frac{d}{d\mu}\left[(1-\mu^2)\frac{dP_\ell}{d\mu}\right] + \ell(\ell+1)P_\ell = 0, \qquad \text{(C.5)}$$

it follows from completeness that

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_\ell}{\partial r}\right) - \frac{\ell(\ell+1)}{r^2}c_\ell + \frac{y_\ell}{D} = 0, \quad \ell = 0,1,2,\ldots . \qquad \text{(C.6)}$$

Expanding the derivatives, Equation (C.6) simplifies to

$$c_\ell'' + \frac{2}{r}c_\ell' - \frac{\ell(\ell+1)}{r^2}c_\ell = -\frac{y_\ell}{D} \qquad \text{(C.7)}$$

The general solutions of the associated homogeneous equation are $f_\ell = r^\ell$ and $g_\ell = r^{-\ell-1}$. Noting the boundary condition at infinity, using the method of variation of parameters (Birkhoff and Rota, 1961), we obtain

$$c_\ell(r) = \frac{1}{r^{\ell+1}} \int_0^r \frac{\rho^{\ell+2} y_\ell(\rho) d\rho}{2\ell+1} + r^\ell \int_r^\infty \frac{y_\ell(\rho) d\rho}{(2\ell+1)\rho^{\ell-1}} . \tag{C.8}$$

The problem thus reduces to a single integral per r value plus a basis set of single integrals over μ per r value. Values of $c(r,\mu)$ at any μ then follow.

We have calculated $c(r,\mu)$ for the case of a concentric elliptical source,

$$y(r,\mu) = Ae^{-\beta r\sqrt{1-\varepsilon^2\mu^2}} \tag{C.9}$$

$$(\varepsilon = \sqrt{1 - 1/b_o^2})$$

The contours of the solution maintain the shape of the source (essentially) near the center, and gradually asymptote towards spherical at large distance.

This behavior may be conveniently represented to a high degree of accuracy by representing $c(r,\mu)$ by the form

$$c(r,\mu) = c(\xi) \tag{C.10}$$

where the generalized radial coordinate, ξ, is defined implicitly by the relation

$$\xi = \sqrt{\rho^2 + (z - z_o)^2/b^2(\xi)} \tag{C.11}$$

where $\rho = r\sqrt{1 - \mu^2}$ and $z = z_o + r\mu$. The function, $b(\xi)$, is the axis ratio parameter of the half-elliptical contour in the ρ-z aximuthal half-plane defined by ξ = constant.

The ξ dependence and the trend in b_o of $b(\xi)$ is interesting. The maximum it approaches--and apparently reaches--at the center is less than b_o and grows sublinearly in b_o-1. If this maximum is stationary, it is so only within a very small ball. The ξ dependence of $b(\xi)$ is very well represented by the exponential form

$$b(\xi) = 1 + \delta e^{-\xi/\xi_b}. \tag{C.12}$$

The dependences of δ and ξ_b on b_o are adequately represented by the forms $\delta = \delta_o(b_o - 1)^p$ and $\xi_b = \xi_{bo} + \xi_{b1}(b_o - 1)$ where $\delta_o = .59$, $p = .83$, $\xi_{bo} = .63$ and $\xi_{b1} = 1.12$. Contour graphs of the approximate solution to the steady state diffusion equation for $b = 2$ are plotted in Fig. (B.1) along with calculated data points.

APPENDIX D
ANALYTIC REPRESENTATION OF STEADY STATE ONE SPECIES TWO BODY DECAY

We present here the derivation of an analytic representation of the steady state solution of one species two body decay. The asymptotic limits we seek to recover are three: (1) pure diffusion as $\kappa/\beta \to 0$, (2) pure localized kinetics as $\kappa/\beta \to \infty$ within the central core, and (3) source independent diffusion kinetic balance in the limb.

The method which suggests itself is to gate between core (pure localized kinetics) and limb (source independent diffusion kinetic balance) for $\kappa/\beta > 0$, and then to gate this expression over to the pure diffusion limit as $\kappa/\beta \to 0$. Since the core is self-gating in κ/β, it is required to gate the limb from the $1/r^2$ diffusion kinetic limit over to the $1/r$ pure diffusion limit.

In actual fact it proved convenient to go about this latter step backwards: one gates to the pure diffusion limit, but not just the pure diffusion limb limit, but the global pure diffusion limit, and then corrects for it in the limb for $\kappa/\beta > 0$, via a gate in r.

The form is given by

$$G = fF_{dk}G_{dif} + g\,G_{kin} \tag{D.1}$$

where

$$G_{dif} = \frac{B}{\beta^3}\left[2(1 - e^{-\beta r}) - \beta r e^{-\beta r}\right] \tag{D.2}$$

$$G_{kin} = \frac{Br}{\kappa^2}[e^{-\beta r/2} - \frac{\beta}{2\gamma} e^{-\gamma r}] \tag{D.3}$$

where

$$\gamma = \frac{g\beta/2\kappa^2}{(\frac{f\kappa^2 + g\beta^2}{\beta^2\kappa^2}) - \frac{C_o}{B}} \tag{D.4}$$

and

$$C_o = B/(\beta^2 + \kappa^2). \tag{D.5}$$

The two choices for the gates are

$$(1) \quad f = (\frac{\beta^2}{\beta^2 + \kappa^2})^p, \; g = (\frac{\kappa^2}{\beta^2 + \kappa^2})^p \tag{D.6}$$

and

$$(2) \quad f = \frac{\beta^{2p}}{\beta^{2p} + \kappa^{2p}}, \; g = \frac{\kappa^{2p}}{\beta^{2p} + \kappa^{2p}}. \tag{D.7}$$

And, finally,

$$F = \frac{1}{1 + \frac{f\kappa^4}{\beta^3}[(r^q + r_o^q)^{1/q} - r_o]} \tag{D.8}$$

where $r_o = r_o'/\beta$.

Certain features of this form deserve explanation.

1. In the limit $\kappa = 0$, $G = G_{dif}$. For $\kappa > 0$, $G \sim 2B/\kappa^4 r$ as $r \to \infty$, taking advantage of the constant term, 2, within brackets in G_{dif}.

2. Since the global diffusion solution is used, which is slope regularized at r=0, and since the factor F is slope regularized at r=0 (for $q > 1$), their product is also. By construction, the difference of exponentials is slope regularized at r=0, irrespective of the value of γ, wherefore the total sum is also.

3. Allowing the opposite gates in κ/β, f and g, to remain completely general for the moment, γ is constructed to regain the result, $C(0) = B/(\beta^2 + \kappa^2)$. The parameter γ does however have a further constraint on it, namely that $\gamma > \beta/2$. This is met by setting $p > 1$ in f and g for either choice of gate.

APPENDIX E
DIFFUSION KINETICS FOR ν BODY DECAY

As an aside of theoretical interest we consider diffusion kinetics for ν-body decay of one species for a continuous source term, turned on at $t = 0$. The equation is given by

$$\frac{\partial c}{\partial t} = \frac{D}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c}{\partial r}\right) - \nu k c^{\nu} + y \tag{E.1}$$

For the spatial dependence of the source term, we use the now familiar exponential form, $y(r) = Ae^{-\beta r} = (\beta^3 Z/8\pi)e^{-\beta r}$, where Z equals the spatially integrated source. In the limit $\beta \to \infty$, $y(r) \to (Z/4\pi)\delta(r)$. The more general form, $w(r) = (\beta^{\nu+3}Z/4\pi\Gamma(\nu+3))r^{\nu}e^{-\beta r}$, where $\nu > 0$, also approaches $(Z/4\pi)\delta(r)$ as $\beta \to \infty$.

The problem in its full time dependent context, specifying zero initial conditions, is well posed. The solution, $c(r,t)$, at earliest times is given by

$$c(r,t) \sim y(r)t \tag{E.2}$$

Although the existence, uniqueness and positive definiteness of the solution at all times, $t > 0$, may be proved by rigorous argument, they are clear from a physical understanding of the equation.

We consider in particular the steady state limit. Setting $c = g/r$, Eq. (E.1) becomes

$$g'' - \frac{\nu k}{D}\left(\frac{g}{r}\right)^{\nu} r = -(\beta^3 Z/8\pi D) r e^{-\beta r} \tag{E.3}$$

Since the steady state limit is the closure of the time dependent solution, one may only argue that it be nonnegative definite. Consider now either the long range limit of the solution for given β or the solution at all $r > 0$ in the limit $\beta \to \infty$. Equation (E.3) then becomes

$$g'' - \frac{\nu k}{D}\left(\frac{g}{r}\right)^{\nu} r = 0 \tag{E.4}$$

for $r > 0$. Substituting $g = g_o r^{\alpha}$ as a trial solution, one obtains the requirements

$$\alpha = \frac{\nu-3}{\nu-1} \quad \text{and} \quad g_o = \left[\frac{2(3-\nu)}{(\nu-1)^2(\nu k/D)}\right]^{\frac{1}{\nu-1}} \tag{E.5}$$

These obviously do not apply to the linear cases $\nu = 0$ and $\nu = 1$ which are covered separately by the well known solutions, $c(r) = Z/Dr$ in the first case and $c(r) = Ze^{-\kappa r}/Dr$, where $\kappa = \sqrt{k/D}$, in the second. Note that $c(r)$ in both of these cases is homogeneous in the source strength, Z.

In all the other cases, the nonlinear ones, this long range solution (or the solution for $r > 0$ in the limit $\beta \to \infty$) is independent of the strength of the source, and is uniquely determined by the equation without boundary conditions, with the exception that we require the solution to decrease to zero as $r \to \infty$. Now, looking at these requirements, we see that, given the trial solution form, the nonzero solution is positive definite only for $0 < \nu < 3$, degenerates to the zero solution for $\nu = 3$ and is in general complex for $\nu > 3$. We

note, however, that for $0 < \nu < 1$, the solution does not decrease to zero as $r \to 0$. This is unacceptable. We note, curiously enough, for the complex cases (i. e. $\nu > 3$) that the modulus of the solution does decrease to zero as $r \to 0$.

Arguing from the analyticity of the form of the equation, we conclude that the only physically acceptable solution which exists in the intervals $0 < \nu < 1$ and $3 < \nu$ is the zero solution. Why this is so appears as something of a mystery from the isolated vantage point of the steady state problem by itself. It should become clear upon considering the full time dependent solution. In this regard the pure kinetic results for general ν may prove relevant. It would be an interesting direction in which to take this thesis work--namely, to expand the capabilities of the computer code, DIFKIN, to calculate for general ν-body kinetic terms.

It is possible to generalize the inverse length, κ, defined in the two-body case to the general ν-body case ($\nu \neq 0, \neq 1$). In the pure kinetic limit, $c(0) = \sqrt[\nu]{A/\nu\kappa}$. If we there set $c(0) = B/\kappa^2$ where $B = A/D$ as was done in the two-body case, then we define an inverse length associated with the problem,

$$\kappa = \left(\frac{D}{A}\left(\frac{A}{\nu\kappa}\right)^{1/\nu}\right)^{1/2} . \tag{E.6}$$

It may prove fruitful to consider the envelope of solutions for constant κ for fixed A and D. It is conjectured that the form $B/(\beta^2 + \kappa^2)$ should again be a reasonably good approximation to $c(0)$. This approximate form looks like a first order result in a Fourier transform space. It should prove interesting to pursue this work further.

APPENDIX F
COMPUTER WORK

In this appendix a library of the major computer programs and data files written or adapted or compiled for or implemented in this thesis are given. They are listed in the order of the chapter or appendix they refer to, and are given in the format of TCP files, in many cases job files with /*include's and JCL. The meaning is generally clear from context and, in most cases, clearer by virtue of displaying in a rather convenient manner program and job organization.

Each chapter section is so indicated by a header. Each TCP file is preceded by a header, giving its name. This is important, since this is how it is referenced in any /*include's appearing in any job files which may include it. Adequate documentation is generally given in each program, explaining the purpose of the program and what is being done in it.

```
------------------------------------------------------------------------------
                                CHAPTER II
------------------------------------------------------------------------------

-----------------------------
            ALPHA
COMMENT:  THIS PROGRAM TAKES AS ITS INPUT OUTPUT OF YH2OSUM
YH2OSUM IS A SLIGHT ADAPTATION OF YH2O WRITTEN BY DANIEL RIO
FOR HIS PH. D. THESIS (1983).
-----------------------------
@@ALPHA JOB (7000,3791,5,5),SCHIPPNICK,CLASS=2
@*PASSWORD
@*ROUTE PRINT LOCAL
@@ EXEC FORTXCG
C
C   MAIN:  READ IN STATE BRANCHING RATIOS--MAP STATES INTO SPECIES
C          1. CALL PREP--READ IN PLUME INTEGRALS
C          2. CALL YLD --CALCULATE SPECIES YIELDS
C          3. WRITE OUT TABLE OF YIELD COMPONENTS AND TOTAL YIELDS
C
      DIMENSION YY(19,4),YF(4)
      DIMENSION NJ(25),ISPECF(25),NJJ(25,19),SPEC(25,19)
      DIMENSION YI(25,1), YIPLUM(25,5), EOX(30), G(25,1)
      DIMENSION GPLUM(25,5)
C
      COMMON/YIELD/ YY,E0,NS,NJ,NJJ,ISPECF,SPEC,YYELEC,XNO
      COMMON/PLUME/ ISW, YI, YIPLUM
C
C   SET ISW: CORRECTION FACTOR IN PLUMES FOR MC COUNTING AGREEMENT
      ISW = 1
C-----------------------------------------------------------------------------
      READ(5,*) IE0
      READ(5,1) (EOX(I),I=1,IE0)
    1 FORMAT(8E10.3)
C
C-----------------------------------------------------------------------------

C READ IN POINTERS FOR PRODUCTION OF VARIOUS SPECIES
C
      NS = 14
C  HARDWIRE THAT IN HERE
C
      DO 209 I=1,NS
C
      READ(2,207) NJ(I),ISPECF(I),(NJJ(I,NN),NN=1,19)
      IF(ISPECF(I).EQ.1) READ(2,208) (SPEC(I,NN),NN=1,10)
C
  209 CONTINUE
C
```

```
C-----------------------------------------------------------------------
C
      WRITE(6,498)
      WRITE(6,499)
C
      DO 520 I=1,NS
C
      NNMAX=NJ(I)
      WRITE(6,500) I,NJ(I),(NJJ(I,NN),SPEC(I,NN),NN=1,NNMAX)
 520  CONTINUE
C
C
C FORMAT STATEMENTS
C
C
 498  FORMAT (' ',///,' STATES WHICH CONTRIBUTE TO PARTICULAR SPECIES')
 499  FORMAT (' '/,T2,' SPECIES',T11,'#STATES',T30,'STATES AND SPECIAL'
     #,' FACTORS')
 500  FORMAT (' '/,T4,I2,T12,I2,3X,10(I2,1X,F5.3,3X))
C
C-----------------------------------------------------------------------
C
C
C LOOP THROUGH ENERGY
      DO 1000 I = 1, IE0
C
C
      CALL PREP
C
      CALL YLD
C
C  WRITE OUT YIELD PLUME COMPONENTS AND TOTAL SUM AND G VALUE
C  AND COMPONENT G VALUES
C
      DO 80 J = 1,15
      G(J,1) = YI(J,1)*100./E0
      DO 78 K = 1,5
      GPLUM(J,K) = YIPLUM(J,K)*100./E0
   78 CONTINUE
C
      WRITE(6,90) J, YI(J,1), (YIPLUM(J,K),K=1,5),
     @                        G(J,1), (GPLUM(J,K),K=1,5)
80    CONTINUE
C
      J = 16
      DO 86 K = 1,3
      YI(J,K) = YI(11,K) + YI(12,K) + YI(13,K)
      G(J,K) = YI(J,K)*100./E0
   86 CONTINUE
      DO 88 K = 1,5
      GPLUM(J,K) = YIPLUM(J,K)*100./E0
```

```
   88 CONTINUE
C
      WRITE(6,90) J, YI(J,1), (YIPLUM(J,K),K=1,5),
     @                        G(J,1), (GPLUM(J,K),K=1,5)
C
C
C
      WRITE(6,95)
 1000 CONTINUE
   90 FORMAT(1H ,I2,2X,1P6E10.3,4X,6E10.3)
   95 FORMAT(1H //)
C
  207 FORMAT (22(I2,1X))
  208 FORMAT (10G5.3)
C
      STOP
      END
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
      SUBROUTINE SFVFL (VAL, VEC, NW)
C
C     SFVFL - STANDARD FORTRAN VECTOR FILL
C
      DIMENSION VEC(1)
      DO 10 I = 1, NW
      VEC(I) = VAL
10     CONTINUE
C
      RETURN
      END
@*INCLUDE ALPHPREP 70003791,1
@*INCLUDE ALPHYILD 70003791,1
@@GO.SYSIN DD *
9
      20.       50.       100.      200.      500.      1000.     3000.     10000.
    30000.
@@GO.FT02F001 DD *
 5  0  8 12 13 14 15
 3  1  7 18 19
1.0  .100 .25
 7  0  8 12 13 14 15 16 17
 0
 6  1  6  9 10 11 18 19
1.   1.   1.   1.   .07  .75
 5  1  6  9 10 11 18
1.   1.   1.   1.   .830
 1  0  7
 0
 0
 0
```

```
 0
 0
 1   1 18
.830
 2   1 18 19
.070 .75
@@GO.FT08F001 DD DSN=JF.B0035006.S1.YNEWSUM,DISP=OLD
@@* DCB=(RECFM=FB,BLKSIZE=6072,LRECL=132)
@@*NEED NOT MENTION, RECORDED IN CATALOG, BUT IF YOU DO, COMMA
@@*MUST GO IN PRECEDING LINE
-----------------------------
              ALPHPREP
COMMENT:  ADAPTATION OF SUBPROGRAM WRITTEN BY RIO
-----------------------------
      SUBROUTINE PREP
C   ..................................................
C   . H2O VERSION :          : H2O SPECIES IS NUMBER 15 .
C   ..................................................
C
      DIMENSION YY(19,4),YF(4)
      DIMENSION NJ(25),ISPECF(25),NJJ(25,19),SPEC(25,19)
      DIMENSION YI(25,1), YIPLUM(25,5)
C
      COMMON/YIELD/ YY,E0,NS,NJ,NJJ,ISPECF,SPEC,YYELEC,XNO
      COMMON/PLUME/ ISW, YI, YIPLUM
C
C
C READ/WRITE OPTION
C
C  15TH SPECIES H2O
C
C     SEE SUBROUTINE BOATYI FOR COMPLETE MAPPING BETWEEN
C     HIS SPECIES LISTING AND MINE
C
C
C CONSTANTS
C
C  NOTE:  RO IS MASS DENSITY IN GM/CC.  DENS IS NUMBER DENSITY IN #/CC
C  DENS NEVER OCCURRED IN HERE ANYWAY
C  NOTE:  10/10/84 NORMALIZE TO RO AND TO RATE.
      RO = 1.
      RO3=RO*RO*RO
      RATE = 1.
C
      AVOG=6.023E+23
C     FCCTOR = 1./AVOG
      FCCTOR = 1.
C  UNITS OF # RATHER THAN MOLES
C
C
```

```
C  BAKGROUND CONC.(H2O) NOT ALLOWED TO VARY
C
C
C INPUT YIELD INFORMATION
C
C READ THE INTEGRATED YY VALUES
C
      DO 190 J=1,19
C
      READ(8,192) E0,IST,(YY(J,I),I=1,4)
C
C  CLEAN UP MYSTERY GARBAGE
      YY(J,4) = 0.
C  OK.
C
  190 CONTINUE
C
C
C  AND WHAT IS MORE, NOW: HUMAN PASS CORRECTION FACTORS TO ALIGN
C  YIELD SPECTRA INTEGRAL COUNTING WITH MONTE CARLO COUNTING
C  CHECK YOU WORK BEFORE YOU GIVE IT TO ME NEXT TIME THANK YOU
C
C  FOR THIS SERIES OF E0 VALUES, XNO(FIT) =
C  1.268,2.330,4.053,7.416,17.21,33.11,94.60,301.2,868.4
C  ACTUAL MONTE CARLO RESULTS ARE
C  -----,2.244,3.822,7.048,16.64,32.89,94.74,300.0,830.0
C
C  NEED IT HERE ALREADY
      XNO = 1.
      IF(E0 .LE. 12.6) GO TO 1113
      XNO = .521 + .0415*E0**.965
 1113 CONTINUE
C
      FAC = 1.
      IF(ISW .EQ. 0) GO TO 444
      IF(E0 .EQ. 20.) FAC = (XNO-1.)/.2272
      IF(E0 .EQ. 50.) FAC = (XNO-1.)/1.354
      IF(E0 .EQ. 100.)FAC = (XNO-1.)/3.145
      IF(E0 .EQ. 200.)FAC = (XNO-1.)/6.840
      IF(E0 .EQ. 500.)FAC = (XNO-1.)/18.21
      IF(E0 .EQ.1000.)FAC = (XNO-1.)/37.27
      IF(E0 .EQ.3000.)FAC = (XNO-1.)/112.4
      IF(E0.EQ.10000.)FAC = (XNO-1.)/367.9
      IF(E0.EQ.30000.)FAC = (XNO-1.)/1077.
  444 CONTINUE
C
      DO 995 J = 16,19
      DO 995 I = 1,2
      YY(J,I) = YY(J,I)*FAC
  995 CONTINUE
```

:

```
C
C
C   J=1 HIGH ENERGY PLUME; J=2 LOW ENERGY PLUME; J=5 DEPOSITION SPECTRUM
C   FROM YNEWSUM DISKFILE
C
C
C
C-----------------------------------------------------------------------
C
      WRITE(6,185) E0,NS
C
C-----------------------------------------------------------------------
C
C
C
C WRITE YIELD INPUT
C
      WRITE(6,195)
      WRITE(6,199)
C
C PROCESS YIELDS
C
       WRITE(6,328)
       WRITE(6,329)
C
      DO 350 J=1,19
C
      DO 320 I=1,4
C
      YF(I)=YY(J,I)*FCCTOR*RATE*RO3
C
C
  320 CONTINUE
C
      WRITE(6,330) (YY(J,I),YF(I),I=1,4)
C
C
      DO 325 I=1,4
C
      YY(J,I)=YF(I)
  325 CONTINUE
  350 CONTINUE
C
C  ELECTRON NORMALIZATION
C  MULTIPLY THE DEPOSITION SPECTRUM BY ELECTRON YIELD
C
      YYELEC=XNO*FCCTOR*RATE*RO3
C
C
      WRITE(6,195)
```

```
C
      RETURN
C
C FORMAT STATEMENTS
C
  2   FORMAT(2A4,2X,G12.5,3X,G12.5)
 192  FORMAT(1X,F8.2,2X,I3,1X,4(1X,G14.7))
 200  FORMAT (5G12.5)
C
 195  FORMAT (' ',//,130('-'))
 199  FORMAT (' ',//,T50,' YIELD INPUT')
C
 185  FORMAT('1',/' ENERGY=',G12.5, 'EV',/,' NUMBER OF SPECIES IS ',
     #I2/1H ,'       (H2O NOT COUNTED)'/)
C
C
C
 328  FORMAT(' ',///,T2,'INTEGRATED YIELD; YY INPUT AND YY*FACTORS'/)
 329  FORMAT(' ',T20,'TERMS 1 -> 3 AND SOURCE')
 330  FORMAT(' ',4(G12.5,1X,G12.5,6X))
C
C
      END
-----------------------------
          ALPHYILD
COMMENT:  ADAPTATION OF SUBPROGRAM WRITTEN BY RIO
-----------------------------
      SUBROUTINE YLD
C
      DIMENSION KI(15), IP(15)
C
C
      DIMENSION YY(19,4),YF(4)
      DIMENSION NJ(25),ISPECF(25),NJJ(25,19),SPEC(25,19)
      DIMENSION YI(25,1), YIPLUM(25,5), ZI(25,5)
C
      COMMON/YIELD/ YY,E0,NS,NJ,NJJ,ISPECF,SPEC,YYELEC,XNO
      COMMON/PLUME/ ISW, YI, YIPLUM
C
      EQUIVALENCE(YIPLUM(1),ZI(1))
C-----------------------------------------------------------------------------
C
C     DATA KI / 1, 7, 2, 15, 5, 4, 6, 8, 3, 13, 12, 11, 10, 14, 9 /
      DATA IP / 2*1, 3*0, 3*1, 1*0, 3*1, 3*0 /
C
      DATA KI / 1,6,2,15,10,9,7,5,8,4,14,13,3,11,12 /
      DATA IP / 3*1, 0, 3*1, 5*0, 2*1, 0 /
C
C****  EXPLANATION IS PERHAPS IN ORDER HERE:
C
```

```
C        DAN                        MY
C
C    1    1 E          1    1    1   E
C    1    2 H2         1    6    2   H
C    1    3 H2O+       1    2    3   H2
C    0    4 H3O+       0   15    4   H2O
C    1    5 OH         0   10    5   HO2
C    1    6 H          0    9    6   H2O2
C    1    7 O          1    7    7   O
C    0    8 O2         1    5    8   OH
C    0    9 H2O2       0    8    9   O2
C    0   10 HO2        0    4   10   H3O+
C    0   11 H+(H2O)2   1   14   11   H+
C    0   12 H+(H2O)3   1   13   12   OH+
C    1   13 OH+        1    3   13   H2O+
C    1   14 H+         0   11   14   H+(H2O)2
        15 H2O         0   12   15   H+(H2O)3
C
C  ON THE LEFT IS DAN'S LIST IN ORDER.  ON THE FAR RIGHT IS MY LIST IN ORDER.
C  MOVING TO THE LEFT FROM MY LIST IS DAN'S CORRESPONDING LIST NUMBER.
C  TO THE LEFT OF THAT IS A 1 OR 0 DEPENDING ON WHETHER THIS SPECIES SHOULD
C  HAVE A NON-ZERO PRIMARY YIELD.  ON THE  F A R  LEFT IS THE LIST OF 1'S AND
C  0'S MAPPING HORIZONTALLY TO DAN'S LIST RATHER THAN TO MINE.  THEREFORE THE
C  ARRAY IP AND ITS USE VIA THE MAPPING ARRAY KI.
C
C  KI GIVES DAN'S LIST NUMBER AS A FUNCTION OF MY LIST NUMBER
C  IP GIVES THE ON-OFF SWITCH AS A FUNCTION OF DAN'S LIST NUMBER
C
C
C
      DO 5 M = 1,25
      DO 4 N = 1,5
4     YIPLUM(M,N) = 0.
      YI(M,1) = 0.
5     CONTINUE
C
C
      I = 1
C
      DO 1500 J = 1, 15
      KIT = KI(J)
      IF(IP(KIT) .EQ. 0) GO TO 1500
C
      YS=0.0
C
      JMAX=NJ(KIT)
      IF (JMAX.EQ.0) GO TO 14
C
      DO 12 II=1,4
C
```

```
      YSADD=0.0
C
      YSUM=0.0
C
      DO 11 JJ=1,JMAX
C  RIU'S BRANCHING RATIO SUM
C
      YADD=0.0
C
      YADD=YY(NJJ(KIT,JJ),II)
      IF(ISPECF(KIT).EQ.1) YADD=YADD*SPEC(KIT,JJ)
C
      YSUM=YSUM+YADD
   11 CONTINUE
C
      YIPLUM(J,II) = YSUM
      YSADD=YSUM
      YS=YS+YSADD
   12 CONTINUE
C
C     YIPLUM(J,3) = YIPLUM(J,1) + YIPLUM(J,4)
C     TO BE USED WITH DISKFILE 'S1.YNEW'
C    FOR DISKFILE 'S1.YNEWSUM' IT IS ALREADY THERE AND SHOULD BE OMITTED
C
C  HERE'S SOMETHING USEFUL TO DO WITH IT, FOR THE ELECTRON, ANYWAY:
C  DECOMP OF STATES SUM AS OPPOSED TO KNOCK ON
C  AND LONG RANGE TOTAL AS OPPOSED TO SHORT (LONG RANGE DECOMP PLUS
C  KNOCK ON
      IF(J .GT. 1) GO TO 44
      YIPLUM(J,3) = YIPLUM(J,1) + YIPLUM(J,2)
      YIPLUM(J,4) = YIPLUM(J,2) + YIPLUM(J,5)
   44 CONTINUE
C
      IF(KIT.NE.1) GO TO 13
C  KIT = 1 FOR THE ELECTRON
C
      YS=YS+YYELEC
      YIPLUM(J,5) = YYELEC
C
   13 CONTINUE
C
      GO TO 20
C
   14 CONTINUE
C
      YS=0
C
   20 CONTINUE
C
C-----------------------
```

```
      YI(J,I) = YS
C-------------------------
 1500 CONTINUE
C
C
C
      YI(2,I) = YI(2,I) + 1.*YI(12,I) + 2.*YI(11,I) + 1.*YI(13,I)
      YI(8,I) = YI(8,I) + 1.102*YI(12,I) + 1.*YI(11,I) + 1.*YI(13,I)
      YI(7,I) = YI(7,I) + .449*YI(12,I)
      YI(1,I) = YI(1,I) - YI(12,I) - YI(11,I) - YI(13,I)
C
      YI(4,I) = -YI(3,I) - .5*(YI(2,I) + YI(8,I))
      YI(1,I) = 0.
C     YI(11,I) = 0.
      YI(12,I) = 0.
      YI(13,I) = 0.
      YI(11,K) = -YI(7,K) - YI(8,K)
C
      DO 333 K = 1,5
      ZI(2,K) = ZI(2,K) + 1.*ZI(12,K) + 2.*ZI(11,K) + 1.*ZI(13,K)
      ZI(8,K) = ZI(8,K) + 1.102*ZI(12,K) + 1.*ZI(11,K) + 1.*ZI(13,K)
      ZI(7,K) = ZI(7,K) + .449*ZI(12,K)
      ZI(1,K) = ZI(1,K) - ZI(12,K) - ZI(11,K) - ZI(13,K)
C
      ZI(4,K) = -ZI(3,K) - .5*(ZI(2,K) + ZI(8,K))
      ZI(1,K) = 0.
C     ZI(11,K) = 0.
      ZI(12,K) = 0.
      ZI(13,K) = 0.
      ZI(11,I) = -ZI(7,I) - ZI(8,I)
  333 CONTINUE
C
C  2 - H    8 - OH    7 - O    1 - E      12 - OH+    11 - H+    13 - H2O+
C  4 - H2O
C
C
C
C
C
C
      RETURN
      END
-----------------------------
*****************************
-----------------------------
              CONTOUR
COMMENT:  THIS CONTOUR PROGRAM ORIGINALLY WRITTEN FOR LAMINAR FLAME CONTOURS
USES ONLY PART OF ITS CAPABILITY HERE
-----------------------------
```

```
@@CONTOUR JOB (2003,5006,50,20),SCHIPPNICK,REGION=750K,CLASS=2
@*PASSWORD
@*ROUTE PRINT LOCAL
@@  EXEC FORTXCG,LPARM='SIZE=750K',PLOT=
C-----------------------------------------------------------------------
C  NOTE   BUG FIXED 8/20/84  FOR CONTOUR GOING BEYOND RMAX
C
C  SEE AT NODE 4
C
C-----------------------------------------------------------------------
      DIMENSION IEXCLL(50,151), IEXCLU(50,151), RCL(50,151), RCU(50,151)
      DIMENSION IPAX(151), RPC(151), TC(50), IB(50), IEL(50), IEU(50)
      DIMENSION R(51), T(51,151), IP(151)
C
      DIMENSION RAX(51), ZAX(151)
      DIMENSION LL(50), LU(50), RCLX(151), RCUX(151)
C
      EQUIVALENCE(R(1),RAX(1))
      DIMENSION Y1(153), XX(153), GR(4000), SYM(50)
C   153 = 151 + 2
C     DIMENSION OF GR SHOULD BE AT LEAST 0.25*IVL*IHL
      COMMON/SCAL/XMAX,XMIN
C
C-----------------------------------
      COMMON /N/ N,I3,FSAV,XLI,XLF,FL
C-----------------------------------
      LOGICAL*1
     X SYM/'A','B','C','D','E','F','G','H','I','J','K','L','M','N','O',
     X     'P','Q','R','S','T','U','V','W','X','Y','Z','1','2','3','4',
     X     '5','6','7','8','9','0','+','=','-','*','@','#','$','%','&',
     X     'A','B','C','D','*'/
C-----------------------------------------------------------------
C
      READ(5,*) IPLOT
C                          IPLOT DETERMINES WHETHER A GOULD PLOT IS
C                          TO BE PRODUCED
C
C     SET MAX NUMBER OF RADIAL POINTS TO BE COMPUTED   -  NR
C     SET MAX NUMBER OF AXIAL POINTS TO BE COMPUTED    -  NZ
      READ(5,*) NZ, NR
      WRITE(6,4919) NZ, NR
C  READ IN WIDTHH, WIDTHV, XMIN, XMAX, RMIN, RMAX
      READ(5,*) WIDTHH, WIDTHV, XMIN, XMAX, RMIN, RMAX
      WRITE(6,*) WIDTHH, WIDTHV, XMIN, XMAX, RMIN, RMAX
C  WIDTH PARAMETERS ARE FOR LATER USE IN THE GOULD PLOT
      ZMAX = XMAX
      ZMIN = XMIN
C-----------------------------------------------------------------
      DR = (RMAX-RMIN)/(NR-1)
```

```
      DO 551 I = 1,NR
  551 RAX(I) = DR*(I-1) + RMIN
C
      DZ = (ZMAX-ZMIN)/(NZ-1)
      DO 552 I = 1,NZ
  552 ZAX(I) = DZ*(I-1) + ZMIN
C
      WRITE(6,1019)
      WRITE(6,1020) (RAX(I),I=1,NR)
      WRITE(6,1019)
 1019 FORMAT(1H0)
      WRITE(6,1020) (ZAX(I), I = 1,NZ)
      WRITE(6,1020)
C-----------------------------------------------------------------
      ITIME = 0
      DO 555 I = 1,NR
      RWW = RAX(I)
      DO 555 J = 1,NZ
      ZWW = ZAX(J)
      T(I,J) = TEMP(RWW,ZWW)
      TIJ = T(I,J)
      IF(ITIME .EQ. 1) WRITE(6,66) RWW,ZWW,TIJ,N,13,FL,FSAV,
     #   XLI,XLF
  555 CONTINUE
   66 FORMAT(1H ,1P3E12.4,I4,I4,2X,2E12.4,2X,2E12.4)
C   SUBROUTINE TEMP USER SUPPLIED * * * * * * * * * * * ** * * * * *
C
      DO 560 J = 1,NZ
      WRITE(6,1020) (T(I,J),I = 1,10)
      WRITE(6,1020) (T(I,J),I = 11,20)
      WRITE(6,1020) (T(I,J),I = 21,30)
      WRITE(6,1020) (T(I,J),I = 31,40)
      WRITE(6,1020) (T(I,J),I = 41,50)
      WRITE(6,1020) T(51,J)
      WRITE(6,1019)
  560 CONTINUE
 1020 FORMAT(1H ,1P10E12.5)
C
C-----------------------------------------------------------------
C  READ IN SCALE FACTOR FOR CONTOUR VALUES
      READ(5,*) TSCAL
      WRITE(6,*) TSCAL
C
C  READ IN NORMALIZED CONTOUR VALUES*****************************************
      READ(5,*) KE
      READ(5,1234) (TC(K),K=1,KE)
 1234 FORMAT(8E10.3)
      WRITE(6,1234) (TC(K),K=1,KE)
C  ***************************************************************
      DO 1222 K = 1,KE
```

```
 1222 TC(K) = TSCAL*TC(K)
      WRITE(6,1234) (TC(K),K=1,KE)
C
C  NODE 0
            DATA IEXCLU,IEXCLL,IPAX/15251*0/,RCU,RCL/15100*0./
C  15251 = 2X50X151 + 151
C
C  NODE 1
C  FIND PEAK, IS IT ON AXIS?
C
      N = 1
C
      NX = NZ
      DO 11 J = 2,NX
      M = 1
      DO 10 I = 2,NR
      IF(T(I,J) .GT. T(M,J)) M = I
 10   CONTINUE
      IP(J) = M
C
C     RPC(J) = R(M,J)
      RPC(J) = R(M)
      N = N + 1
      IF(M .NE. 1) GO TO 11
C  REGIONS 4 AND 5
      N = N - 1
      IPAX(J) = 1
C
   11 CONTINUE
      IPXT = N
      IPXE = AMIN0(NZ, N + 1)
C
C     IPXT IS THE AXIAL STATION AT WHICH THE PEAK CONTOUR MEETS THE AXIS
C
C  IPNZ=1 IF PEAK CONTOUR HAS NOT YET REACHED AXIS BY STATION NZ
      IPNZ=0
      IF(IP(NZ).GT.1)IPNZ=1
C
C  NODE 2
      DO 29 K = 1,KE
      TK = TC(K)
      ICPXT = 0
      TEND = T(1,IPXT)
      IF(IPNZ.EQ.1)TEND=T(IP(NZ),NZ)
      IF(TK .GT. TEND) ICPXT = 1
C  L-CONTOUR NEEDS NO SPECIAL TREATMENT IF CONTOUR RECONNECTS ON RIGHT
      DO 30 J = 2,NX
      IPJ = IP(J)
      TPJ = T(IPJ,J)
C
```

```
C       RPJ = R(IPJ,J)
        RPJ = R(IPJ)
C
        IPX = IPAX(J)
C
        IF(TK .LE. TPJ) GO TO 21
C   CONTOUR VALUE .GT. PEAK VALUE -- REGIONS 1 AND 5
        RCU(K,J) = RPJ
        RCL(K,J) = RPJ
C   OPTION TO COALESCE CONTOURS WITH PEAK CONTOUR  BOTH FOR PEAK ON AND OFF
C   AXIS
        IEXCLU(K,J) = 1
        IEXCLL(K,J) = 1
C   NOTE: IEXCLL IS NOT FINISHED. REGION 3 AWAITS (HANDLED IN NODE 3)
C
   21 CONTINUE
C
C   NODE 3
        IF(ICPXT .EQ. 1) GO TO 17
C   NOW FINISH OFF IEXCLL  (THE EXCITEMENT BUILDS )
C
        IF(IPJ .NE. 1 .AND. TK .GE. T(1,J)) GO TO 17
C   1ST INEQ. DESCRIBES REG. 1 & 2 AND ALL BUT END PT. OF REG. 3
C   2ND INEQ. DESCRIBES REG. 1,2,5 AND ONLY ONE END PT. OF REG. 4
C   INTERSECTION IS UNION OF REGIONS 1 AND 2.
C   COMPLEMENT IS UNION OF REGIONS 3, 4 AND 5.
C
        IEXCLL(K,J) = 1
        RCL(K,J) = 0.
   17 CONTINUE
C
C   NOW TAKE CARE OF EXTERIOR CONTOURS
C
C   NODE 4
        NRM1 = NR - 1
        DO 15 I = IPJ,NRM1
        M = I
        IF(TK .GE. T(I+1,J)) GO TO 16
   15 CONTINUE
C       WRITE(6,1090) K, TK, J, T(NR,J)
C1090 FORMAT(1H ,'TC(',I2,') = ',F8.3,' .LT. T(NR,',I3,') = ',F8.3)
C   T(NR,J) SAME VALUE FOR ALL J.  TK .LT. THIS VALUE SHOULD NOT BE CHOSEN.
C
C    WHAT?      8/20/84   FIX FOR CONTOUR GOING BEYOND RMAX
C
        RCU(K,J) = R(M+1)
C-----------*****----------*****-----------*****-----------*****-----------
C
        GO TO 101
   16 CONTINUE
```

```
C
C       RCU(K,J) = (R(M,J) + R(M+1,J))/2.
        RCU(K,J) = (R(M) + R(M+1))/2.
C
        TDM = T(M+1,J) - T(M,J)
        IF(TDM .EQ. 0.) GO TO 9901
        RAT = (TK - T(M,J))/(T(M+1,J) - T(M,J))
C
C       RCU(K,J) = R(M,J) + RAT*(R(M+1,J) - R(M,J))
        RCU(K,J) = R(M) + RAT*(R(M+1) - R(M))
C
 9901 CONTINUE
C   ASSIGN CONTOUR POINT IN INTERVAL BETW. RADIAL GRID PTS M AND M+1
C
  101 CONTINUE
C
C   NOW GO ON TO INTERIOR POINTS
C   NODE 5
C
        IPJM1 = IPJ - 1
        DO 25 I = 1,IPJM1
        IL = IPJ - I
        M = IL
        IF(TK .GE. T(IL,J)) GO TO 26
   25 CONTINUE
C
C   TK = TC(K) .LT. T(1,J)
C
        GO TO 102
   26 CONTINUE
C
C       RCL(K,J) = (R(M,J) + R(M+1,J))/2.
        RCL(K,J) = (R(M) + R(M+1))/2.
C
        TDM = T(M+1,J) - T(M,J)
        IF(TDM .EQ. 0.) GO TO 9902
        RAT = (TK - T(M,J))/(T(M+1,J) - T(M,J))
C
C       RCL(K,J) = R(M,J) + RAT*(R(M+1,J) - R(M,J))
        RCL(K,J) = R(M) + RAT*(R(M+1) - R(M))
C
 9902 CONTINUE
C   ASSIGN CONTOUR POINT IN INTERVAL BETW. RADIAL GRID PTS M AND M+1
C   SINCE CONC. GRADIENT IS POSITIVE IN INTERIOR REGION, T DECREASES AS
C   INDEX IL = IPJ - I DESCENDS
C
  102 CONTINUE
   30 CONTINUE
C
C   NODE 6
```

:

```
C   ASSIGNMENTS OF RCL AND RCU EITHER THRU AXIS OR PEAK CONTOUR COALESCENCE
C   ASSIGNMENT OR THRU INTERPOLATION.
C
C   NOW FIND 1ST 0 VALUE OF IEXCLL AND IEXCLU (SAME FOR BOTH?)   --  IB
C   AND LAST 0 VALUE -- IEL AND IEU.
      DO 31 J = 2,NX
      M = J
      IF(IEXCLU(K,J) .EQ. 0) GO TO 32
C
   31 CONTINUE
   32 CONTINUE
      IB(K) = M
      IF(M .LE. 2)GO TO 132
C   UNLESS THESE CONCENTRATIONS ARE INITIALIZED AT THE NOZZLE LIP AS NONZERO
C   THEN .EQ. 1 OK
      IB(K) = M - 1
      RCU(K,M-1) = RPC(M-1)
      RCL(K,M-1) = RPC(M-1)
  132 CONTINUE
C   SEE COMMENT IN TEMP. PROGRAM
C
      DO 33 J = M,NX
      N = J
      IF(IEXCLL(K,J) .EQ. 1) GO TO 34
   33 CONTINUE
   34 CONTINUE
      IEL(K) = N
      IF(IEL(K).EQ.NZ)GOTO2034
      RCL(K,IEL(K)) = RPC(IEL(K))
      IF(ICPXT.EQ.0)RCL(K,IEL(K))=0.
C   ICPXT=0 IMPLIES TK .LT(IN FACT .LE.). TEND.
 2034 CONTINUE
C
      DO 35 J = M,NX
      N = J
      IF(IEXCLU(K,J) .EQ. 1) GO TO 36
   35 CONTINUE
   36 CONTINUE
      IEU(K) = N
C   DITTO
      IF(IEU(K).EQ.NZ)GOTO2036
      RCU(K,IEU(K)) = RPC(IEU(K))
      IF(ICPXT.EQ.0)RCU(K,IEU(K))=0.
 2036 CONTINUE
C
   29 CONTINUE
C-----------------------------------------------------------------------
C
C   GOULD PLOT AND GRAPHING ROUTINE
C
```

```
      IGRAPH = 1
C     IPLOT READ IN AT BEGINNING OF PROGRAM
C     WIDTHH, WIDTHV, XMIN, XMAX, RMIN, RMAX ALSO
C   IF IPLOT=1 MAKES GOULD PLOT
C   IF IGRAPH=1 MAKES GRAPH FOR EACH CONTOUR
C
C
      IVL = 81
      IHL = 101
      IVLH = IVL/4
      IHLH = IHL/4
C
C   SET SCALE FOR GRAPH
C
C   NOTE ZAX(J) FROM UNIT 8 IS IN UNITS OF RJ
      DX = XMAX - XMIN
      XNP1 = XMIN
      XNP2 = DX/WIDTHH
C
      PRINT 3500,DX
      PRINT 4488,NZ,KE
 4488 FORMAT(4I4)
C
C
C   SET SCALES FOR BOTH AXES OF GRAPH AND STARTING VALUES.
C
      DR = RMAX - RMIN
      RNP1 = RMIN
      RNP2 = DR/WIDTHV
C
C   INITIALIZE PLOT
C
      WIH = WIDTHH + 1.05E0
      WIV = WIDTHV + 1.05E0
C
      IF(IPLOT.EQ.1)CALL PLOTS(WIH,WIV,0,1,1.,1.)
      IF(IPLOT.EQ.1)CALL LINEWT(-1)
C     IF(IGRAPH.EQ.1)PRINT 7741
C7741 FORMAT(1H1)
      IF(IGRAPH.EQ.1)CALL PLOT1(1,IVL,IVLH,IHL,IHLH)
      IF(IPLOT.EQ.1)CALL AXIS(0.,0.,'X',-1,WIDTHH,0.0,XNP1,XNP2)
      IF(IPLOT.EQ.1)CALL AXIS(0.,0.,'R', 1,WIDTHV,90.,RNP1,RNP2)
      IF(IPLOT.EQ.1)CALL PLOT(0.,WIDTHV,3)
      IF(IPLOT.EQ.1)CALL PLOT(WIDTHH,WIDTHV,2)
      IF(IPLOT.EQ.1)CALL PLOT(WIDTHH,0.,2)
      IF(IGRAPH.EQ.1)CALL PLOT2(GR,XMAX,XMIN,RMAX,RMIN)
C
C   THE FRAME IS NOW SET UP
C
C
```

```
C- - - - - - - - - - - - - - - - - - - - - - - - - - -
      DO 400 K = 1,KE
C
C  MAP THE CONTOUR INDEX INTERVAL TO A CORRESPONDING ONE BEGINNING AT 1
C
      LL(K) = IEL(K) - IB(K) + 1
      LU(K) = IEU(K) - IB(K) + 1
C
      LLX = LL(K)
      LUX = LU(K)
C
C     LUX = AMAX0(LLX,LUX)
C
      DO 310 L = 1,LUX
      J = IB(K) + L - 1
      RCLX(L) = RCL(K,J)
      RCUX(L) = RCU(K,J)
      XX(L) = ZAX(J)
  310 CONTINUE
C
C
C
      NZMOD = LUX
      IE = IEU(K)
      DO 390 I2 = 1,2
      IF(NZMOD .LE. 1) GO TO 380
C
C  FIRST DO EXTERIOR (U) CONTOURS, THEN INTERIOR ONES (L)
C
      NZ1 = NZMOD + 1
      NZ2 = NZMOD + 2
      XX(NZ1) = XNP1
      XX(NZ2) = XNP2
      YI(NZ1) = RNP1
      YI(NZ2) = RNP2
      PRINT 3500, XX(NZ1),XX(NZ2),K,IB(K),IE,NZMOD,XX(1),XX(NZMOD)
     1 ,YI(NZ1),YI(NZ2)
 3500 FORMAT(10X,1P2E13.4,4I6,1P4E13.4)
C
      DO 330 J = 1,NZMOD
      COC = RCUX(J)
      IF(I2.EQ.2) COC = RCLX(J)
C- - - - - - - - - - - - - - - - - - - - - - - - - - -
      IF(COC.GT.RMAX)COC = -1.E-8 + RMAX
      IF(COC.LT.RMIN)COC =  1.E-8 + RMIN
      YI(J) = COC
C- - - - - - - - - - - - - - - - - - - - - - - - - - -
  330 CONTINUE
C
C  PLOT ARRAY
```

```
C
      IF(IPLOT.EQ.1)CALL LINE(XX,Y1,NZMOD,1,0)
      IF(IGRAPH.EQ.1)CALL PLOT3(SYM(K),XX(1),Y1(1),NZMOD)
C
  380 CONTINUE
      IE = IEL(K)
      NZMOD = LLX
  390 CONTINUE
  400 CONTINUE
C
C  NOW PLOT THE PEAK CONTOUR
C
      IF(IPXE .LE. 2) GO TO 345
      DO 350 L = 2,IPXE
      XX(L-1) = ZAX(L)
  350 CONTINUE
C
      IPXM = IPXE - 1
      NZ1 = IPXM + 1
      NZ2 = IPXM + 2
      XX(NZ1) = XNP1
      XX(NZ2) = XNP2
      Y1(NZ1) = RNP1
      Y1(NZ2) = RNP2
      PRINT 1033, XX(NZ1),XX(NZ2),IPXM,XX(1),XX(IPXM),Y1(NZ1),
     1            Y1(NZ2)
 1033 FORMAT(1H ,1P2E13.4,I6,1P4E13.4)
C
C
      DO 340 J =2,IPXE
      COC = RPC(J)
C- - - - - - - - - - - - - - - - - - - - - -
      IF(COC.GT.RMAX)COC = -1.E-8 + RMAX
      IF(COC.LT.RMIN)COC =  1.E-8 + RMIN
      Y1(J-1) = COC
C- - - - - - - - - - - - - - - - - - - - - -
  340 CONTINUE
C
C  PLOT ARRAY
C
      IF(IPLOT.EQ.1)CALL LINE(XX,Y1,IPXM,1,0)
      IF(IGRAPH.EQ.1)CALL PLOT3(SYM(50),XX(1),Y1(1),IPXM)
  345 CONTINUE
C
      IF(IPLOT.EQ.1)CALL PLOT(0.,0.,999)
      IF(IGRAPH.EQ.1)CALL PLOT4(2,2HR )
C
      DO 4090 K = 1,KE
      WRITE(6,4919)(IEXCLL(K,J),J=1,NX)
      WRITE(6,4919)(IEXCLU(K,J),J=1,NX)
```

```
      WRITE(6,4920)(RCL(K,J),J=1,NX)
      WRITE(6,4920)(RCU(K,J),J=1,NX)
 4090 WRITE(6,4921)IB(K),IEL(K),IEU(K),TC(K)
      WRITE(6,4919)(IPAX(J),J=1,NX),IPXE
      WRITE(6,4919)(IP(J),J=1,NX)
      WRITE(6,4920)(RPC(J),J=1,NX)
      WRITE(6,1235) (T(IP(J),J),J=1,NX)
C
C
 9444 CONTINUE
C
 1235 FORMAT(1H ,1P12E11.3)
 4919 FORMAT(1H ,20I6)
 4920 FORMAT(1H ,20F6.3)
 4921 FORMAT(1H ,3I6,1PE10.3)
      STOP
      END
@*INCLUDE CON.TEMP   70003791,1
1
151  51
10. 5. -1.E-7  1.E-7  0.  1.E-7
1.
10
 1.0000E20 5.0000E19 2.0000E19 1.0000E19 5.0000E18 2.0000E18 1.0000E18 5.0000E17
 2.0000E17 1.0000E17
@@ EXEC PLOT
-------------------------------
          CON.TEMP
COMMENT:  SPATIAL YIELD SPECTRA ANALYTIC REPRESENTATION AS GIVEN IN CHAPTER
TWO ENCODED HERE
-------------------------------
      FUNCTION TEMP(R,Z)
      REAL KK
C
      DATA PI/ 3.141593/
C     DATA CC0, CC2, XL/ .0282, 902., 3.21/
C     NOT NEEDED
C
      DATA AA, BB, PP, EE, KK/ 1.37E7, 2.65E-5, 1.75, .197, 4.56/
      DATA C1, C2, Q1, Q2/ 4.05E-2, 6.16E-6, 0.543, 1.88/
C     DATA C1, C2, Q1, Q2/ 2.25E-2, 1.34E-5, 0.662, 1.88/
      DATA EEEE, PPPP, QQQQ/ 251., 48.2, 90.6/
      DATA ALPHA, EEGG, EESS, SIG/ 0.751, 185., 407., 736./
C
      DATA DENSGM, E0, E/ 1., 1000., 910./
C
      BET = AA/(E0**EE + BB*E0**PP)
      BETS = KK*AA/(E0**EE + KK*BB*E0**PP)
      ZOP = C1*E0**Q1 + C2*E0**Q2
      ZOP = 1.8E-7*ZOP
```

```
C  REFERENCE MASS DENSITY
      XXX = PPPP*ALUG(E0/EEEE + 1.)
      EPS = (XXX/(XXX + 1.))**QQQQ
      GAMINF = SQRT(1. - EPS*EPS)
      GAMLOW = 1. + ALPHA*E0/EEGG*EXP(-E0/EEGG)
      GAMFAC = (1.-GAMINF)*(SIG+1.)/(SIG+EXP(E0/EESS)) + GAMINF
      GAM = GAMLOW*GAMFAC
C
      AAAA = (1. - EPS*EPS)**2*GAM*GAM*BET*BET*BET/8./PI
      AAAAS = AAAA*BETS*BETS*BETS/BET/BET/BET
C
      RD = R*DENSGM
      ZD = Z*DENSGM
C
      SQ = SQRT(GAM*GAM*RD*RD + (ZD - Z0P)*(ZD - Z0P))
      ARG = BET*(SQ - EPS*(ZD - Z0P))
      ARGS = BETS/BET*ARG
      GGGG = EXP(-ARG)
      GGGGS = EXP(-ARGS)
C
      BETE = AA/(E**EE + BB*E**PP)
      F = BET/BETE
C
      TEMP = F*AAAAS*GGGGS + (1. - F)*AAAA*GGGG
C
      RETURN
      END
-----------------------------
*****************************
-----------------------------
```

CHAPTER III AND APPENDIX D

```
-----------------------------
            RUN.SP
-----------------------------
@@GREENFCN JOB (2003,5006,130,5,0),'PAUL SCHIPPNICK',CLASS=T
@*PASSWORD
@*ROUTE PRINT LOCAL
@@  EXEC FORTXCG
@@SYSPRINT DD DUMMY
@*INCLUDE GN.MSP
@*INCLUDE UT.SMSON
@*INCLUDE FCN.SP
@*INCLUDE UT.VM2D
@@GO.SYSIN DD *
5.1E0   4.0E-14   0.282E0   40.E0
-----------------------------
```

GN.MSP

```
C
C     THIS PROGRAM CALCULATES THE SOLUTION TO THE RADIAL DIFFUSION EQUATION
C     OVER A GRID IN R AND T BY MEANS OF THE GREEN'S FUNCTION KERNEL INTEGRAL
C     -- A TWO DIMENSIONAL INTEGRAL OVER R0 AND T0...
C
C     ...OR A ONE DIMENSIONAL INTEGRAL OVER T0 FOR T < TC WHERE TC =
C     (520 - 10*R)/D.
C
C
C     THESE POINTS ARE THEN INTERPOLATED BETWEEN USING A SIMPSON'S RULE
C     SUBROUTINE IN ORDER TO GENERATE A FINER GRID OF POINTS AT A CHEAPER
C     COST.
C
C     THESE POINTS ARE THEN TABULATED AND PLOTTED USING THE GOULD PLOTTER.
C
C     AS IN THE DIFFUSION KINETICS CODE (ADAPTED BOAT) THE GRID IN R IS
C     EVENLY SPACED IN LN(R+1).  A LOGARITHMIC GRID IN T IS ALSO USED.
C
C
      DIMENSION RR(50), RLR(50), TT(30), RRI(200), RLRI(200)
      DIMENSION U(30,50), UI(30,200), BUF1(50), BUF2(200)
      DIMENSION E(30,50)
C
      COMMON / PARAM / R, D, B
      COMMON / RRRR / RRRR
C
      EXTERNAL FUN2, FN1D
      CALL ERRSET(208,2000,1,-1)
C
C
      IX = 15
      JX = 11
      RLRX = 5.0
C
      IFF = 2
C
C     NOTE: IFF CAN BE 1,2,3, OR 4.  4 IS PRESENTLY THE MAX VALUE.
C     PER THE DIMENSIONING OF THE ARRAY UI.
C
      JXI = 1 + IFF*(JX-1)
C
      EPS = 1.E-2
      PI = 3.14159265358979323846264 3
      READ(5,*) D, A, B, RRRR
      SQRTPD = SQRT(PI*D)
C
C     IT MAY BE ADVISABLE TO MAKE RRRR DEPEND ON R AND T SOMEHOW.
```

```
C
C
C
C
C
C
      DATA TT / 2.E-3, 5.E-3, 1.E-2, 2.E-2, 5.E-2, 1.E-1, 2.E-1, 5.E-1,
     1          1.E-0, 2.E-0, 5.E-0, 1.E+1, 2.E+1, 5.E+1, 1.E+2, 2.E+2,
     2          5.E+2, 1.E+3, 2.E+3, 5.E+3, 10*1.E+4 /
C
      DATA TT / .01, .03, .1, .3, 1., 3., 10., 30., 100., 300., 1000.,
     1          3000., 10000., 30000., 100000., 15*300000. /
C
C
      DO 10 J = 2, JX
      RLR(J) = RLRX*(J-1)/(JX-1)
   10 RR(J) = EXP(RLR(J)) - 1.E0
C
      DO 20 J = 2, JXI
      RLRI(J) = RLRX*(J-1)/(JXI-1)
   20 RRI(J) = EXP(RLRI(J)) - 1.E0
C
C  GUARD AGAINST DIVIDE CHECK IF R = 0.  IN EFFECT CALCULATE THE L'HOPITAL
C  LIMIT.  FUN1(R0,TAU) = FUN1(R0,TAU;R,T), TAU = T - T0, HAS DENOMINATOR
C  OF R.
C
      RR(1) = EPS
      RRI(1) = EPS
      RLR(1) = EPS
      RLRI(1) = EPS
C
C
      DO 30 I = 1, IX
C
      T = TT(I)
      EPSTTT = 1.E-7*T
      IF (EPSTTT .GT. 1.E-7) EPSTTT = 1.E-7
      BEG = EPSTTT
      NP1 = 32
      NP2 = 32
      IF ( I .EQ. 1) GO TO 90
      BEG = TT(I-1)
      NP1 = 24
      NP2 = 24
   90 CONTINUE
C
      DO 29 J = 1, JX
      R = RR(J)
      TOL = 0.E0
      ITAG = 0
C
      TC = (520.E0 - 0.1E0*R)/D
      IF(TC .LT. 0.E0) TC = 0.E0
C
```

```
      IF(T .GT. TC) GO TO 91
      U(I,J) = A/2.E0/R*VM1D(TOL, BEG, T, FN1D, ERRE, 0, 9, NP1)
      E(I,J) = A/2.E0/R*ERRE
      GO TO 93
   91 CONTINUE
      ITAG = 1
      U(I,J) = 0.5E0*A/SQRTPD/R*VM2D(TOL,BEG,T,FUN2,ERRE,0,9,NP2)
      E(I,J) = 0.5E0*A/SQRTPD/R*ERRE
   93 CONTINUE
      USAVE = U(I,J)
      ESAVE = E(I,J)
      IF(I .EQ. 1) GO TO 92
      U(I,J) = U(I,J) + U(I-1,J)
      E(I,J) = E(I,J) + E(I-1,J)
   92 CONTINUE
C
      WRITE(6,2099) I, J, R, RLR(J), T, U(I,J), E(I,J),
     X   USAVE, ESAVE, ITAG
C
   29 CONTINUE
   30 CONTINUE
 2099 FORMAT(1H , 2I3, 1P7D12.5,I5)
C
C
C
C
C
C
C
C
C  INTERPOLATE THE RESULTS
C
      IF (IFF .EQ. 1) GO TO 41
      DO 40 I = 1, IX
C
      DO 31 J = 1, JX
      BUF1(J) = U(I,J)
      IF(BUF1(J) .LE. 0.E0) BUF1(J) = 1.E-40
   31 BUF1(J) = ALOG(BUF1(J))
C
      CALL SIMSON( RLR, BUF1, RLRI, BUF2, JX, JXI, 0)
C
      DO 32 J = 1, JXI
   32 UI(I,J) = EXP(BUF2(J))
C
   40 CONTINUE
   41 CONTINUE
C
C
C
```

```
      IXMOD = IX/10
      IXTRUN = IXMOD*10
      IPAGE = IXMOD
      IF (IXTRUN .NE. IX) IPAGE = IXMOD + 1
C
      DO 200 I = 1, IPAGE
      ISTART = 1 + (I-1)*10
      IEND = ISTART + 9
      IF(IEND .GT. IX) IEND = IX
      WRITE(6,101)
      WRITE(6,102) (TT(II), II = ISTART,IEND)
      DO 180 J = 1, JXI
  180 WRITE(6,103) RRI(J), RLRI(J), (UI(II,J), II = ISTART,IEND)
  200 CONTINUE
C
C
      IXMOD = IX/5
      IXTRUN = IXMOD*5
      IPAGE = IXMOD
      IF (IXTRUN .NE. IX) IPAGE = IXMOD + 1
C
      DO 300 I = 1, IPAGE
      ISTART = 1 + (I-1)*5
      IEND = ISTART + 4
      IF(IEND .GT. IX) IEND = IX
      WRITE(6,101)
      WRITE(6,202) (TT(II), II = ISTART,IEND)
      DO 280 J = 1, JX
  280 WRITE(6,203) RR(J), RLR(J), (U(II,J), E(II,J), II = ISTART,IEND)
  300 CONTINUE
C
  101 FORMAT(1H1,'TIME DEPENDENT RADIAL DIFFUSION PROBLEM WITH SOURCE TE
     1RM TURNED ON AT T= 0. I.C.=0 EVERYWHERE. B.C. U=0 AT R=INFINITY.'/
     2/50X,'C(R,T) IN MOLE/CC'/)
  102 FORMAT(1H0,10HR (CM)     10HLN(R+1)    11HT (SEC) =  /1H ,20X,1P10D1
     $1.3/)
  202 FORMAT(1H0,10HR (CM)     10HLN(R+1)    11HT (SEC) =  /1H ,20X,
     $ 1PE11.3,11X,E11.3,11X,E11.3,11X,E11.3,11X,E11.3,11X/)
  103 FORMAT(1H ,1P2E10.3,  10E11.4)
  203 FORMAT(1H ,1P2E10.3, E11.4,'+/-',E8.2, E11.4,'+/-',E8.2, E11.4,'+/
     $-',E8.2, E11.4,'+/-',E8.2, E11.4,'+/-',E8.2)
C
C
      STOP
      END
-----------------------------
            GN.MSP1
-----------------------------
C
C  THIS PROGRAM CALCULATES THE SOLUTION TO THE RADIAL DIFFUSION EQUATION
```

```
C     OVER A GRID IN R AND T BY MEANS OF THE GREEN'S FUNCTION KERNEL INTEGRAL
C     -- A TWO DIMENSIONAL INTEGRAL OVER RO AND TO...
C
C     ...OR A ONE DIMENSIONAL INTEGRAL OVER TO FOR T < TC WHERE TC =
C     (520 - 10*R)/D.
C
C
C     THESE POINTS ARE THEN INTERPOLATED BETWEEN USING A SIMPSON'S RULE
C     SUBROUTINE IN ORDER TO GENERATE A FINER GRID OF POINTS AT A CHEAPER
C     COST.
C
C     THESE POINTS ARE THEN TABULATED AND PLOTTED USING THE GOULD PLOTTER.
C
C     AS IN THE DIFFUSION KINETICS CODE (ADAPTED BOAT) THE GRID IN R IS
C     EVENLY SPACED IN LN(R+1).  A LOGARITHMIC GRID IN T IS ALSO USED.
C
      DIMENSION RR(50), RLR(50), TT(30), RRI(200), RLRI(200)
      DIMENSION U(30,50), UI(30,200), BUF1(50), BUF2(200)
      DIMENSION E(30,50)
C
      COMMON / PARAM / R, D, B
      COMMON / RRRR / RRRR
C
      EXTERNAL FUN2, FN1D
      CALL ERRSET(208,2000,1,-1)
C
C
      IX = 13
      JX = 6
C
      IFF = 2
C
C     NOTE: IFF CAN BE 1,2,3, OR 4.  4 IS PRESENTLY THE MAX VALUE.
C     PER THE DIMENSIONING OF THE ARRAY UI.
C
      JXI = 1 + IFF*(JX-1)
C
      EPS = 1.D-7
      PI = 3.14159265358979323846264 3
      READ(5,*) D, A, B, RRRR
      SQRTPD = SQRT(PI*D)
C
C     IT MAY BE ADVISABLE TO MAKE RRRR DEPEND ON R AND T SOMEHOW.
C
C
C
      DATA TT / 2.E-3, 5.E-3, 1.E-2, 2.E-2, 5.E-2, 1.E-1, 2.E-1, 5.E-1,
C    1          1.E-0, 2.E-0, 5.E-0, 1.E+1, 2.E+1, 5.E+1, 1.E+2, 2.E+2,
C    2          5.E+2, 1.E+3, 2.E+3, 5.E+3, 10*1.E+4 /
```

:

```
C
      DATA TT / .01, .03, .1, .3, 1., 3., 10., 30., 100., 300., 1000.,
     1          3000., 18*10000. /
C
C
C
C*************************************************************************
C
C
      DATA RR / 1.E-6,1.E-5,1.E-4,1.E-3,1.E-2,1.E-1, 44*1.E0 /
C
      DO 10 J = 1, JX
      RLR(J) = ALOG(RR(J))
   10 CONTINUE
C
      RLRX = RLR(JX)
C
      DO 20 J = 2, JXI
      RLRI(J) = RLRX*(J-1)/(JXI-1)
   20 RRI(J) = EXP(RLRI(J))
C
C*************************************************************************
C
      DO 30 I = 1, IX
C
      T = TT(I)
      EPSTTT = 1.E-7*T
      IF (EPSTTT .GT. 1.E-7) EPSTTT = 1.E-7
      BEG = EPSTTT
      NP1 = 32
      NP2 = 32
      IF (I .EQ. 1) GO TO 90
      BEG = TT(I-1)
      NP1 = 24
      NP2 = 24
   90 CONTINUE
C
      DO 29 J = 1, JX
      R = RR(J)
      TOL = 0.E0
      ITAG = 0
C
      TC = (520.E0 - 0.1E0*R)/D
      IF(TC .LT. 0.E0) TC = 0.E0
C
      IF(T .GT. TC) GO TO 91
      U(I,J) = A/2.E0/R*VM1D(TOL, BEG, T, FN1D, ERRE, 0, 9, NP1)
      E(I,J) = A/2.E0/R*ERRE
      GO TO 93
   91 CONTINUE
```

```
      ITAG = 1
      U(I,J) = 0.5E0*A/SQRTPD/R*VM2D(TOL,BEG,T,FUN2,ERRE,0,9,NP2)
      E(I,J) = 0.5E0*A/SQRTPD/R*ERRE
   93 CONTINUE
      USAVE = U(I,J)
      ESAVE = E(I,J)
      IF(I .EQ. 1) GO TO 92
      U(I,J) = U(I,J) + U(I-1,J)
      E(I,J) = E(I,J) + E(I-1,J)
   92 CONTINUE
C
      WRITE(6,2099) I, J, R, RLR(J), T, U(I,J), E(I,J),
     X   USAVE, ESAVE, ITAG
C
   29 CONTINUE
   30 CONTINUE
 2099 FORMAT(1H , 2I3, 1P7D12.5,I5)
C
C
C
```

```
      ISTART = 1 + (I-1)*10
      IEND = ISTART + 9
      IF(IEND .GT. IX) IEND = IX
      WRITE(6,101)
      WRITE(6,102) (TT(II), II = ISTART,IEND)
      DO 180 J = 1, JXI
  180 WRITE(6,103) RRI(J), RLRI(J), (UI(II,J), II = ISTART,IEND)
  200 CONTINUE
C
C
      IXMOD = IX/5
      IXTRUN = IXMOD*5
      IPAGE = IXMOD
      IF (IXTRUN .NE. IX) IPAGE = IXMOD + 1
C
      DO 300 I = 1, IPAGE
      ISTART = 1 + (I-1)*5
      IEND = ISTART + 4
      IF(IEND .GT. IX) IEND = IX
      WRITE(6,101)
      WRITE(6,202) (TT(II), II = ISTART,IEND)
      DO 280 J = 1, JX
  280 WRITE(6,203) RR(J), RLR(J), (U(II,J), E(II,J), II = ISTART,IEND)
  300 CONTINUE
C
  101 FORMAT(1H1,'TIME DEPENDENT RADIAL DIFFUSION PROBLEM WITH SOURCE TE
     1RM TURNED ON AT T= 0. I.C.=0 EVERYWHERE. B.C. U=0 AT R=INFINITY.'/
     2/50X,'C(R,T) IN MOLE/CC'/)
  102 FORMAT(1H0,10HR (CM)     10HLN(R+1)    11HT (SEC) =  /1H ,20X,1P10D1
     $1.3/)
  202 FORMAT(1H0,10HR (CM)     10HLN(R+1)    11HT (SEC) =  /1H ,20X,
     $ 1PE11.3,11X,E11.3,11X,E11.3,11X,E11.3,11X,E11.3,11X/)
  103 FORMAT(1H ,1P2E10.3,  10E11.4)
  203 FORMAT(1H ,1P2E10.3, E11.4,'+/-',E8.2, E11.4,'+/-',E8.2, E11.4,'+/
     $-',E8.2, E11.4,'+/-',E8.2, E11.4,'+/-',E8.2)
C
C
      STOP
      END
-----------------------------
            FCN.SP
-----------------------------
      FUNCTION FN1D(TOL,TAU,ERRE)
      IMPLICIT REAL*16 (A-H,O-Z)
      REAL*4 TOL, TAU, ERRE, R, D, B, FN1D
      COMMON / PARAM / R, D, B
C
C  NOTE:  THE FORTRAN LIBRARY FUNCTION ERF(X), DERF(X) = 2/SQRT(PI)*INTEGRAL
C  FROM 0. TO X OF EXP(-U*U)*DU.  DEFINITIONS OF ERFC AND DERFC ARE CONSIS-
C  TENT WITH THIS.  AT LARGE VALUES OF X, AN ASYMPTOTIC EXPANSION IS USED TO
```

```
C   CALCULATE ERF HERE INSTEAD OF CALLING THE FORTRAN LIBRARY FUNCTION.  THIS
C   IS DONE SO THAT AN OVERFLOW EXPONENTIAL APPEARING AS A FACTOR ALONG WITH
C   THE EXPRESSION (1. + ERF) CAN BE CANCELLED OUT.
C
      RR = R
      DD = D
      BB = B
      TTAU = TAU
C
      SQPI = 1.772453850905516027298167
C
      AP = -2.Q0*DD*TTAU*BB + RR
      AM = -2.Q0*DD*TTAU*BB - RR
      C = 4.Q0*DD*TTAU
      SQC = QSQRT(C)
C
      SQCOPI = SQC/SQPI
C
      APSQC = AP/SQC
      AMSQC = AM/SQC
      VAPSQC = QABS(APSQC)
      VAMSQC = QABS(AMSQC)
C
      IF ( VAPSQC .GT. 12.70 ) GO TO 11
      TERM1 = AP*QEXP((AP*AP-RR*RR)/C)*(1.Q0 + QERF(APSQC))
      GO TO 12
   11 CONTINUE
C
      TERM = 1.Q0
      SUM = 1.Q0
      DO 100 I = 1, 25
      TERM = -1.Q0*TERM*(2.Q0*I-1.Q0)/2.Q0/APSQC/APSQC
  100 SUM = SUM + TERM
C
      TERM1 = -SQCOPI*QEXP(-RR*RR/C)*SUM
      IF(AP .GT. 0.Q0) TERM1 = TERM1 + 2.Q0*AP*QEXP((AP*AP-RR*RR)/C)
C23456789 123456789 123456789 123456789 123456789 123456789 123456789 1234567890
   12 CONTINUE
      IF (VAMSQC .GT. 12.70´) GO TO 13
      TERM2 = AM*QEXP((AM*AM-RR*RR)/C)*(1.Q0 + QERF(AMSQC))
      GO TO 14
   13 CONTINUE
C
      TERM = 1.Q0
      SUM = 1.Q0
      DO 200 I = 1, 25
      TERM = -1.Q0*TERM*(2.Q0*I-1.Q0)/2.Q0/AMSQC/AMSQC
  200 SUM = SUM + TERM
C
      TERM2 = -SQCOPI*QEXP(-RR*RR/C)*SUM
```

```
   14 CONTINUE
      FN1D = TERM1 - TERM2
      ERRE = 1.E-25
      RETURN
      END
      FUNCTION FUN1 ( TOL, R0, ERRE )
C
      COMMON / PASS / TAU
      COMMON / RRRR / RRRR
      COMMON / PARAM / R, D, B
C
C     A = 4.0E-14     B = 0.282
C
C
C  UNITS: (A) = MOLE/CC/SEC     (B) = 1/CM
C
C
C  F(R0) = 4*PI*RHO(R0) = SOURCE TERM = A*EXP(-B*R0)
C
C
C
C  INTEGRAL OVER R0 FROM 0 TO INFINITY = SUM OF INTEGRAL FROM 0 TO RRRR
C  PLUS INTEGRAL FROM RRRR TO INFINITY.  IN LATTER INTEGRAL TRANSFORM FROM
C  R0 TO S0 = RRRR**2/R0.  THIS INTEGRAL = INTEGRAL FROM 0 TO RRRR OF
C  RRRR**2/R0**2*F(RRRR**2/R0), OR IN TERMS OF S0 = S0(R0), S0/R0*F(S0).
C
C  GUARD AGAINST UNDERFLOW OF EXPONENTIAL ARGUMENT AT R0 = 0
C
      DEN = 4.E0*D*TAU
C
C
C
C     TERM1 = R0*(EXP(-B*R0-(R-R0)**2/DEN)-EXP(-B*R0-(R+R0)**2/DEN))
C
      TERM2 = 0.E0
      IF( R0 .EQ. 0.E0) GO TO 10
      S0 = RRRR*RRRR/R0
      TERM2 = S0*(EXP(-B*S0-(R-S0)**2/DEN)-EXP(-B*S0-(R+S0)**2/DEN))
      TERM2 = S0/R0*TERM2
   10 CONTINUE
      FUN1 = (TERM1 + TERM2)
      ERRE = 1.E-7
      RETURN
      END
      FUNCTION FUN2(TOL,TAU,ERRE)
      COMMON / PASS / PTAU
      COMMON / RRRR / RRRR
      EXTERNAL FUN1
      PTAU = TAU
      FUN2 = VM1D(TOL, 0.E0, RRRR, FUN1, ERRE, 0, 9, 32)
      FUN2 = FUN2/SQRT(TAU)
      RETURN
      END
```

```
------------------------------
*****************************
------------------------------
              RUN.CHEM
------------------------------
@@GRENCHEM JOB (2003,5006,400,10,0),'PAUL SCHIPPNICK',CLASS=1
@*PASSWORD
@*ROUTE PRINT LOCAL
@@  EXEC FORTXCG
@*INCLUDE GN.CHEM
@*INCLUDE FCN.CHEM
@*INCLUDE UT.VM2D
@@GO.SYSIN DD *
1141.
.894E-14    .2639    .233E-15    .6390    1859.
.755E-13    .2639    .225E-14    .6390    1829.
6.294E12
1.
1141.
2.60E-14    1.330    1.50E-12    1.330    1859.
2.01E-13    1.330    1.15E-11    1.330    1829.
6.294E12
.15
------------------------------
              RUN.CHMX
------------------------------
@@GRENCHEM JOB (2003,5006,400,10,0),'PAUL SCHIPPNICK',CLASS=1
@*PASSWORD
@*ROUTE PRINT LOCAL
@@  EXEC FORTXCG
@*INCLUDE GN.CHMX
@*INCLUDE FCN.CHEM
@*INCLUDE UT.VM2D
@@GO.SYSIN DD *
1141.
2.60E-14    1.330    1.50E-12    3.375    1859.
2.01E-13    1.330    1.15E-11    3.375    1829.
6.294E12
1.
------------------------------
              GN.CHEM
------------------------------
C
C   THIS PROGRAM CALCULATES THE SOLUTION TO THE RADIAL DIFFUSION EQUATION
C   OVER A GRID IN R AND T BY MEANS OF THE GREEN'S FUNCTION KERNEL INTEGRAL
C   -- A TWO DIMENSIONAL INTEGRAL OVER RO AND TO...
C
C
C
C   THESE POINTS ARE THEN INTERPOLATED BETWEEN USING A SIMPSON'S RULE
```

```
C     SUBROUTINE IN ORDER TO GENERATE A FINER GRID OF POINTS AT A CHEAPER
C     COST.
C
C     THESE POINTS ARE THEN TABULATED AND PLOTTED USING THE GOULD PLOTTER.
C
C     AS IN THE DIFFUSION KINETICS CODE (ADAPTED BOAT) THE GRID IN R IS
C     EVENLY SPACED IN LN(R+1).  A LOGARITHMIC GRID IN T IS ALSO USED.
C
C
      DIMENSION RR(50), TT(30), U(30,50), E(30,50)
C
      COMMON / PARAM / R, T, D, FF
      COMMON /SOURCE/ A1, B1, AP1, BP1, D1,  A2, B2, AP2, BP2, D2
C
      EXTERNAL FUN2
      CALL ERRSET(208,2000,1,-1)
      CALL ERRSET(207,2000,1,-1)
C
C
      IS = 4
      IX = 26
      JX = 8
C
C
C
      PI = 3.14159265358979323846264 3
      READ(5,*)  D, A1, B1, AP1, BP1, D1, A2, B2, AP2, BP2, D2
      READ(5,*) REACRA
      READ(5,*) FF
      WRITE(6,*)D, A1, B1, AP1, BP1, D1, A2, B2, AP2, BP2, D2
      WRITE(6,*) REACRA
      WRITE(6,*) FF
C
      SQRTPD = SQRT(PI*D)
C
C
C
C
      DATA TT / .00003,
     W          .0001, .0003, .001, .003,
     X          .01, .03, .1, .3, 1., 3., 10.,  100.,  1000.,
     1          10000.,  100000., 1.E6, 1.E7, 1.E8, 1.E9, 1.E10,
     2          1.E11, 1.E12, 1.E13, 1.E14, 1.E15, 5*1.E15 /
C
C
C
C     AS RR--> 0 L'HOPITAL LIMIT IS CALCULATED.  BREAKS DOWN TOO CLOSE.
```

```
C   .01 FOR B = .26 IS STARTING TO BECOME INACCURATE.
C
C
      DATA RR/ 1., 2., 5., 10., 20., 35., 50., 70./
C
C     DO 999 I = 1,IX
C 999 RR(I) = RR(I)/10.
C
C
C
C
      DO 29 J = 1, JX
      R = RR(J)
C
      DO 30 I = IS, IX
C
      T = TT(I)
      BEG = 0.
      END = 0.9999999*T
C  SINGLE PRECISION ZERO GUARD FOR TAU = T - T0
      NP1 = 32
      NP2 = 32
      IF (I .EQ. 1) GO TO 90
      BEG = TT(I-1)
      NP1 = 24
      NP2 = 24
   90 CONTINUE
C
      TOL = 0.E0
      U(I,J) = 0.5E0/SQRTPD/R*VM2D(TOL,BEG,END,FUN2,ERRE,0,9,NP2)
      E(I,J) = 0.5E0/SQRTPD/R*ERRE
      U(I,J) = REACRA*U(I,J)
      E(I,J) = REACRA*E(I,J)
      USAVE = U(I,J)
      ESAVE = E(I,J)
      IF(I .EQ. 1) GO TO 92
      U(I,J) = U(I,J) + U(I-1,J)
      E(I,J) = E(I,J) + E(I-1,J)
   92 CONTINUE
C
      WRITE(6,2099) I, J,  R, T, U(I,J), E(I,J),
     X   USAVE, ESAVE
C
   30 CONTINUE
   29 CONTINUE
 2099 FORMAT(1H , 2I3, 1P10D12.5)
C
C
C
C
```

```
C
C
C
C
      IXMOD = IX/10
      IXTRUN = IXMOD*10
      IPAGE = IXMOD
      IF (IXTRUN .NE. IX) IPAGE = IXMOD + 1
C
      DO 200 I = 1, IPAGE
      ISTART = 1 + (I-1)*10
      IEND = ISTART + 9
      IF(IEND .GT. IX) IEND = IX
      WRITE(6,101)
      WRITE(6,102) (TT(II), II = ISTART,IEND)
      DO 180 J = 1, JX
  180 WRITE(6,103) RR(J),  (U(II,J), II = ISTART,IEND)
  200 CONTINUE
C
C
      IXMOD = IX/5
      IXTRUN = IXMOD*5
      IPAGE = IXMOD
      IF (IXTRUN .NE. IX) IPAGE = IXMOD + 1
C
      DO 300 I = 1, IPAGE
      ISTART = 1 + (I-1)*5
      IEND = ISTART + 4
      IF(IEND .GT. IX) IEND = IX
      WRITE(6,101)
      WRITE(6,202) (TT(II), II = ISTART,IEND)
      DO 280 J = 1, JX
  280 WRITE(6,203) RR(J),  (U(II,J), E(II,J), II = ISTART,IEND)
  300 CONTINUE
C
  101 FORMAT(1H1,'TIME DEPENDENT RADIAL DIFFUSION PROBLEM WITH SOURCE TE
     1RM TURNED ON AT T= 0. I.C.=0 EVERYWHERE. B.C. U=0 AT R=INFINITY.'/
     2/50X,'C(R,T) IN MOLE/CC',/)
  102 FORMAT(1H0,10HR (CM)     10H                    11HT (SEC) =  /1H ,20X,1P10D1
     $1.3/)
  202 FORMAT(1H0,10HR (CM)     10H                    11HT (SEC) =  /1H ,20X,
     $ 1PE11.3,11X,E11.3,11X,E11.3,11X,E11.3,11X,E11.3,11X/)
  103 FORMAT(1H ,1PE10.3,  10E11.4)
  203 FORMAT(1H ,1PE10.3, E11.4,' +-',E8.2, E11.4,' +-',E8.2, E11.4,'+/
     $-',E8.2, E11.4,' +-',E8.2, E11.4,' +-',E8.2)
C
C
      STOP
      END
-----------------------------
```

GN.CHMX

```
C
C   THIS PROGRAM CALCULATES THE SOLUTION TO THE RADIAL DIFFUSION EQUATION
C   OVER A GRID IN R AND T BY MEANS OF THE GREEN'S FUNCTION KERNEL INTEGRAL
C   -- A TWO DIMENSIONAL INTEGRAL OVER R0 AND T0...
C
C
C
C
C   THESE POINTS ARE THEN INTERPOLATED BETWEEN USING A SIMPSON'S RULE
C   SUBROUTINE IN ORDER TO GENERATE A FINER GRID OF POINTS AT A CHEAPER
C   COST.
C
C   THESE POINTS ARE THEN TABULATED AND PLOTTED USING THE GOULD PLOTTER.
C
C   AS IN THE DIFFUSION KINETICS CODE (ADAPTED BOAT) THE GRID IN R IS
C   EVENLY SPACED IN LN(R+1).  A LOGARITHMIC GRID IN T IS ALSO USED.
C
C
      DIMENSION RR(50), TT(30), U(30,50), E(30,50)
C
      COMMON / PARAM / R, T, D, FF
      COMMON /SOURCE/ A1, B1, AP1, BP1, D1,  A2, B2, AP2, BP2, D2
C
      EXTERNAL FUN2
      CALL ERRSET(208,2000,1,-1)
      CALL ERRSET(207,2000,1,-1)
C
C
      IS = 1
      IX = 23
      JX = 8
C
C
C
C
      PI = 3.14159265358979323846264 3
      READ(5,*)  D, A1, B1, AP1, BP1, D1, A2, B2, AP2, BP2, D2
      READ(5,*) REACRA
      READ(5,*) FF
      WRITE(6,*)D, A1, B1, AP1, BP1, D1, A2, B2, AP2, BP2, D2
      WRITE(6,*) REACRA
      WRITE(6,*) FF
C
      SQRTPD = SQRT(PI*D)
C
C
C
C
```

```
      DATA TT / .00003,
     W          .0001, .0003, .001, .003,
     X          .01, .03, .1, .3, 1., 3., 10.,  100.,  1000.,
     1          10000.,  100000., 1.E6, 1.E7, 1.E8, 1.E9, 1.E10,
     2          1.E11, 1.E12, 1.E13, 1.E14, 1.E15, 5*1.E15 /
C
C
C
C
C  AS RR--> 0 L'HOPITAL LIMIT IS CALCULATED.  BREAKS DOWN TOO CLOSE.
C  .01 FOR B = .26 IS STARTING TO BECOME INACCURATE.
C
C
      DATA RR/ 1., 2., 5., 10., 20., 35., 50., 70./
C
      DO 999 I = 1,IX
  999 RR(I) = RR(I)/10.
C
C
C
C
      DO 29 J = 1, JX
      R = RR(J)
C
      DO 30 I = IS, IX
C
      T = TT(I)
      BEG = 0.
      END = 0.9999999*T
C  SINGLE PRECISION ZERO GUARD FOR TAU = T - TO
      NP1 = 32
      NP2 = 32
      IF (I .EQ. 1) GO TO 90
      BEG = TT(I-1)
      NP1 = 24
      NP2 = 24
   90 CONTINUE
C
      TOL = 0.E0
      U(I,J) = 0.5E0/SQRTPD/R*VM2D(TOL,BEG,END,FUN2,ERRE,0,9,NP2)
      E(I,J) = 0.5E0/SQRTPD/R*ERRE
      U(I,J) = REACRA*U(I,J)
      E(I,J) = REACRA*E(I,J)
      USAVE = U(I,J)
      ESAVE = E(I,J)
      IF(I .EQ. 1) GO TO 92
      U(I,J) = U(I,J) + U(I-1,J)
      E(I,J) = E(I,J) + E(I-1,J)
   92 CONTINUE
C
```

```
      WRITE(6,2099) I, J,  R, T, U(I,J), E(I,J),
     X   USAVE, ESAVE
C
   30 CONTINUE
   29 CONTINUE
 2099 FORMAT(1H , 2I3, 1P10D12.5)
C
C
C
C
C
C
C
      IXMOD = IX/10
      IXTRUN = IXMOD*10
      IPAGE = IXMOD
      IF (IXTRUN .NE. IX) IPAGE = IXMOD + 1
C
      DO 200 I = 1, IPAGE
      ISTART = 1 + (I-1)*10
      IEND = ISTART + 9
      IF(IEND .GT. IX) IEND = IX
      WRITE(6,101)
      WRITE(6,102) (TT(II), II = ISTART,IEND)
      DO 180 J = 1, JX
  180 WRITE(6,103) RR(J),  (U(II,J), II = ISTART,IEND)
  200 CONTINUE
C
C
      IXMOD = IX/5
      IXTRUN = IXMOD*5
      IPAGE = IXMOD
      IF (IXTRUN .NE. IX) IPAGE = IXMOD + 1
C
      DO 300 I = 1, IPAGE
      ISTART = 1 + (I-1)*5
      IEND = ISTART + 4
      IF(IEND .GT. IX) IEND = IX
      WRITE(6,101)
      WRITE(6,202) (TT(II), II = ISTART,IEND)
      DO 280 J = 1, JX
  280 WRITE(6,203) RR(J),  (U(II,J), E(II,J), II = ISTART,IEND)
  300 CONTINUE
C
  101 FORMAT(1H1,'TIME DEPENDENT RADIAL DIFFUSION PROBLEM WITH SOURCE TE
     1RM TURNED ON AT T= 0. I.C.=0 EVERYWHERE. B.C. U=0 AT R=INFINITY.'/
     2/50X,'C(R,T) IN MOLE/CC'/)
  102 FORMAT(1H0,10HR (CM)     10H              11HT (SEC) =  /1H ,20X,1P10D1
     $1.3/)
```

```
  202 FORMAT(1H0,10HR (CM)     10H            11HT (SEC) =  /1H ,20X,
     $ 1PE11.3,11X,E11.3,11X,E11.3,11X,E11.3,11X,E11.3,11X/)
  103 FORMAT(1H ,1PE10.3,  10E11.4)
  203 FORMAT(1H ,1PE10.3, E11.4,' +-',E8.2, E11.4,' +-',E8.2, E11.4,'+/
     $-',E8.2, E11.4,' +-',E8.2, E11.4,' +-',E8.2)
C
C
      STOP
      END
-----------------------------
*****************************
-----------------------------
            CYL1
-----------------------------
C   THIS PROGRAM CALCULATES THE SOLUTION TO THE DIFFUSION EQUA-
C   TION FOR CYLINDRICALLY SYMMETRIC SOURCE FUNCTION AND INIT-
C   IAL CONDITION. U(RHO,Z;0) = 0., BOUNDARY CONDITION, U = 0.
C   AT INFINITY.
C
C   --OVER A GRID IN R, THETA AND T BY A GREEN'S FUNCTION INTE-
C   GRAL OVER R0, MU0, PHI0 AND T0 IN THE ORDER PHI0, MU0, R0,
C   T0.
C
C   THE INTEGRAL OVER PHI0 IS ANALYTIC AND IS EVALUATED AS SUCH.
C   --MODIFIED BESSEL FUNCTION ORDER 0
C
C   A GRID IN R, THETA RATHER THAN IN RHO,Z IS USED IN ORDER TO
C   TAKE ADVANTAGE OF THE GEOMETRY OF THE SYSTEM FOR THE SAKE OF
C   OPTIMAL UTILIZATION.
C
C   BOB COLDWELL'S VARIABLE MESH MULTIPLE INTEGRATION PROGRAM,
C   VM-N-D IS USED.
C
C   THESE POINTS CAN THEN BE INTERPOLATED BETWEEN IN R AND IN
C   THETA.  THE LOG-LOG GRAPH OF U VERSUS R IS INFLECTION FREE,
C   THEREFORE A SIMPSON'S RULE INTERPOLATION SUFFICES.  THE
C   DEPENDENCE ON THETA BETWEEN 0 AND PI/2 AND IN ANY OF THE
C   OTHER THREE QUADRANTS IS A SINUSOIDAL-LIKE "GATE" BETWEEN
C   TWO VALUES SEPARATED BY A SMALL RELATIVE DIFFERENCE.
C     THEREFORE A SIMPSON'S RULE SUFFICES FOR THIS.
C
C
C
C
C
      REAL*4 MU
      DIMENSION RR(21), RLR(21), TT(15), RRI(081), RLRI(081)
      DIMENSION THETA(11), THETAI(11), U(15,21,11), UI(15,081,11)
      DIMENSION BUF1(21), BUF2(081), E(15,21,11)
```

```
      COMMON / PARAM / R, D, B, BZ, MU
      COMMON / RRRR / RRRR
      COMMON / NP / NP
C
      EXTERNAL FUN4
C
C
      READ(5,*)  IS,JS,KS, IX,JX,KX, RLRX, IFF
      WRITE(6,*)  IS,JS,KS, IX,JX,KX, RLRX, IFF
C
C
C  NOTE: IFF CAN BE 1,2,3, OR 4.  4 IS PRESENTLY THE MAX VALUE.
C  PER THE DIMENSIONING OF THE ARRAY UI.
C
      JXI = 1 + IFF*(JX-1)
C
      EPS = 1.E-2
C-----------------------------------
C     PI = 3.14159265358979323846264 3
C-----------------------------------
      PI = 3.141592654
      READ(5,*) D, A, B, RRRR, BZ
      CALL CLOSE(5)
C NECESSARY ON VAX IN ORDER TO RUN TWO OR MORE JOBS CONCURRENTLY
C WHICH ARE READING FROM THE SAME UNIT FILE
C
      BI = 1./B
      COEF = 2.*PI/8./(PI*D)**1.5
C  FACTOR OF 2*PI FROM PHI INTEGRAL NORMALIZED FACTOR
      ECC = SQRT(1. - 1./BZ/BZ)
C  THE ECCENTRICITY, NORMALLY SYMBOLIZED BY EPSILON
C
      WRITE(6,*) D, A, B, BI, RRRR, BZ, ECC
      B = BI
C
C  IT MAY BE ADVISABLE TO MAKE RRRR DEPEND ON R AND T SOMEHOW.
C  YOU BETTER BELIEVE IT
C
C
C     DATA TT / 2.E-3, 5.E-3, 1.E-2, 2.E-2, 5.E-2, 1.E-1, 2.E-1, 5.E-1,
C    1          1.E-0, 2.E-0, 5.E-0, 1.E+1, 2.E+1, 5.E+1, 1.E+2, 2.E+2,
C    2          5.E+2, 1.E+3, 2.E+3, 5.E+3, 10*1.E+4 /
C
C     DATA TT / .01, .03, .1, .3, 1., 3., 10., 30., 100., 300., 1000.,
C    1          3000., 10000., 30000., 100000. /
      DATA TT/.01,.1,1.,10.,100.,1000.,10000.,100000.,7*1000000./
C
C
      DO 10 J = 2, JX
      RLR(J) = RLRX*(J-1)/(JX-1)
```

```
   10 RR(J) = EXP(RLR(J)) - 1.E0
C
      DO 20 J = 2, JXI
      RLRI(J) = RLRX*(J-1)/(JXI-1)
   20 RRI(J) = EXP(RLRI(J)) - 1.E0
C
C  GUARD AGAINST DIVIDE CHECK IF R = 0.  IN EFFECT CALCULATE THE L'HOPIT
C  LIMIT.  FUN1(R0,TAU) = FUN1(R0,TAU;R,T), TAU = T - T0, HAS DENOMINATO
C  OF R.
C
      RR(1) = EPS
C     RRI(1) = EPS
C     RLR(1) = EPS
C     RLRI(1) = EPS
C  NO SWEAT --  THIS ISN'T THE TWO AND ONE DIMENSIONAL INTEGRAL
C  OF SPHERICAL FAME
C
C
CCCC
```

```
C
      T = TT(I)
      EPSTTT = 1.E-7*T
      IF (EPSTTT .GT. 1.E-7) EPSTTT = 1.E-7
      BEG = EPSTTT
      IF (I .EQ. IS) GO TO 90
      BEG = TT(I-1)
   90 CONTINUE
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C-.-.-.
```

```
C   THAT'S IT
C
C   NOT EVERYTHING, NOw I DO SOMETHING BOB COLDWELL TOLD ME
C   NOT TO DO, ROGUE THAT I AM
C
C   HERE WE CALCULATE THE ASYMPTOTICALLY EARLY ANALYTIC LIMIT
C   OF THE SOLUTION, AND USE IN PLACE OF THE NUMERICAL GREEN'S
C   FUNCTION INTEGRAL WE ARE ATTEMPTION TO CALCULATE HERE IF
C   IT FAILS BECAUSE IT COULDN'T FIND A NARROW PEAK
C     I CAN MODIFY THE PROGRAM LATER TO MAKE IT SMART ABOUT
C     LOCATING THAT PEAK BUT I CAN'T AFFORD THE TIME RIGHT NOW
C   SO THERE
C
C   UND WIR HABEN ABER NICHT AUF UNSERE KOEPFE GEFALLEN DA
C   WIR SEHR KLUG SIND, WIR WISSEN DASS WIR ES DA EBEN BESSER
C   MACHEN KOENNEN WENN WIR DIE SPLINEFORMEL DAZU BENUTZEN
C   UM NOCH EINEN HOEHEREN RANG DES REALISMUS ZU ERLANGEN.
C     DAS HEISST NUR SO DA DIE FRUEHERE EFFEKTE DER DIFFUSION
C   DIE SIND RADIALERWEISE HER, ALSO FOLGT DER ELLIPTISCHE
C   FALL FRUEHERER ZEIT AUF EINER ANALOGEN WEISE MIT DEM
C   SPHAERISCHEN.
C
C   THAT IS ALL
C
      ELL = SQRT(1. - (ECC*MU)**2)
      ASTSAV = AST
      XP = RP*ELL
      TPP = TP/(1. + .56*(4.*TP/(XP*XP + 1.97))**.65)
      COP = TP/(1. + 1.4*TP**.5 + TP)
      GAT = EXP(-XP*XP/4./TPP)
      FAT = GAT
      EE = EXP(-XP)
      CSTP   = 1.
      IF(XP .EQ. 0.) GO TO 1400
      CSTP = 2.*(1. - EE)/XP - EE
 1400 CONTINUE
      CP = CSTP*COP*FAT + (1.-FAT)*((1.-GAT)*TPP + GAT*COP)*EE
      AST = A*CP/D/B/B
      ASTDIF = AST - ASTSAV
C
C-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-
C
C
      U(I,J,K) = COEF*A*VM4D(TOL,BEG,T,FUN4,ERRE,0,9,NP)
      E(I,J,K) = COEF*A*ERRE
C  EMPLOY QUICK AND DIRTY FIX RIGHT HERE
      ALARM = .001*ESTDIF
C  RECALL ESTDIF IS A MINIMUM ESTIMATE SINCE IT GOES FOR
C  THE CIRCLE INSCRIBED IN THE ELLIPSE, FURTHERMORE, THE
C  SPLINE UNDERESTIMATES FOR THE MOST PART WHERE IT DEVI-
```

```
C  ATES, PERIOD SO AT EARLY TIMES, AT LONG TIMES NEAR
C  STEADY STATE IT MAY OVERESTIMATE SLIGHTLY, SO WHAT
C
C  THEREFORE IF THE CALCULATED VALUE IS EVEN 0.1*ESTDIF
C  CHANCES ARE EXCELLENT THAT THE PEAK HAS NOT BEEN LOCATED
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C  THAT'S NOT TRUE
C
C  IT'S FEAST OR FAMINE   ALL OR NOTHING
C
C  IF IT GOT THAT BIG AND DIDN'T GO ALL THE WAY THEN
C  WOW
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C    MINIMUM ESTIMATE OF INSCRIPTION BECAUSE THE LONGER
C    LIMB OF THE ELLIPTICAL DISTRIBUTION WILL BE SENDING
C    (DIFFUSING) STUFF OVER TO THE SHORTER LIMB
C
      IF(U(I,J,K) .LE. ALARM) ITAG = 1
      IF(ITAG .EQ. 1) U(I,J,K) = ASTDIF
      IF(ITAG .EQ. 1) ERRE = 0.
C
      USAVE = U(I,J,K)
      ESAVE = E(I,J,K)
      IF(I .EQ. 1) GO TO 92
      U(I,J,K) = U(I,J,K) + U(I-1,J,K)
      E(I,J,K) = E(I,J,K) + E(I-1,J,K)
   92 CONTINUE
C
      WRITE(6,2099) I, J, K, R, RLR(J), T, THET, U(I,J,K), E(I,J,K),
     X   USAVE, ESAVE, AST, ASTDIF, ITAG
C
   30 CONTINUE
      WRITE(6,3334)
   28 CONTINUE
      WRITE(6,3333)
   29 CONTINUE
      WRITE(6,3333)
      WRITE(6,3333)
 2099 FORMAT(1H , 3I3, 1P10D12.5,I2)
C
 3333 FORMAT(1H0)
 3334 FORMAT(1H0//)
C
C
C
C
```

```
C
C
C   INTERPOLATE THE RESULTS
C
C   SKIP IF EITHER JS OR KS IS NOT EQUAL TO 1
      IF(JS .NE. 1  .OR.  KS .NE. 1) GO TO 500
C
C
      IF (IFF .EQ. 1) GO TO 41
      DO 40 I = 1, IX
      DO 39 K = 1, KX
C
      DO 31 J = 1, JX
      BUF1(J) = U(I,J,K)
      IF(BUF1(J) .LE. 0.E0) BUF1(J) = 1.E-35
   31 BUF1(J) = ALOG(BUF1(J))
C
      CALL SIMSON( RLR, BUF1, RLRI, BUF2, JX, JXI, 0)
C
      DO 32 J = 1, JXI
   32 UI(I,J,K) = EXP(BUF2(J))
C
   39 CONTINUE
   40 CONTINUE
   41 CONTINUE
C
C
C
      IXMOD = IX/10
      IXTRUN = IXMOD*10
      IPAGE = IXMOD
      IF (IXTRUN .NE. IX) IPAGE = IXMOD + 1
C
      DO 400 K = 1, KX
C
      DO 200 I = 1, IPAGE
      ISTART = 1 + (I-1)*10
      IEND = ISTART + 9
      IF(IEND .GT. IX) IEND = IX
      WRITE(6,101)  THETA(K)
      WRITE(6,102) (TT(II), II = ISTART,IEND)
      DO 180 J = 1, JXI
  180 WRITE(6,103) RRI(J), RLRI(J), (UI(II,J,K), II = ISTART,IEND)
  200 CONTINUE
C
C
      IXMOD = IX/5
      IXTRUN = IXMOD*5
      IPAGE = IXMOD
      IF (IXTRUN .NE. IX) IPAGE = IXMOD + 1
```

```
C
      DO 300 I = 1, IPAGE
      ISTART = 1 + (I-1)*5
      IEND = ISTART + 4
      IF(IEND .GT. IX) IEND = IX
      WRITE(6,101) THETA(K)
      WRITE(6,202) (TT(II), II = ISTART,IEND)
      DO 280 J = 1, JX
  280 WRITE(6,203) RR(J), RLR(J), (U(II,J,K), E(II,J,K), II=ISTART,IEND)
C23456789 123456789 123456789 123456789 123456789 123456789 123456789 12
  300 CONTINUE
  400 CONTINUE
  500 CONTINUE
C
  101 FORMAT(1H0,'TIME DEPENDENT DIFFUSION PROBLEM WITH SOURCE TURNED ON
     $ AT T = 0, I.C.=0 EVERYWHERE, B.C. U=0 AT R=INFINITY.'/1H0,'THETA
     $= ',F6.3//1H ,'C(R,THETA,T) IN MOLE/CC'/1H0,
     $'THETA = ',F9.4,' DEG'//)
  102 FORMAT(1H0,10HR (CM)     10HLN(R+1)    11HT (SEC) =  /1H ,20X,1P10D1
     $1.3/)
  202 FORMAT(1H0,10HR (CM)     10HLN(R+1)    11HT (SEC) =  /1H ,20X,
     $ 1PE11.3,11X,E11.3,11X,E11.3,11X,E11.3,11X,E11.3,11X/)
  103 FORMAT(1H ,1P2E10.3,  10E11.4)
  203 FORMAT(1H ,1P2E10.3, E11.4,'+/-',E8.2, E11.4,'+/-',E8.2, E11.4,'+/
     $-',E8.2, E11.4,'+/-',E8.2, E11.4,'+/-',E8.2)
C
C
      STOP
      END
@*INCLUDE UT.SMBBL 20035006,12
      FUNCTION FUN4(TOL,TAU,ERRE)
      COMMON / PASS / PTAU
      COMMON / RRRR / RRRR
      COMMON / NP / NP
      EXTERNAL FUN3
      PTAU = TAU
      FUN4 = VM3D(TOL, 0.E0, RRRR, FUN3, ERRE, 0, 9, NP)
      FUN4 = FUN4/TAU**1.5
      ERRE = ERRE/TAU**1.5
      RETURN
      END
--------------------------------
                CYL2
COMMENT:  THIS INCLUDES BOB COLDWELL'S VARIABLE MESH INTEGRATION ROUTINE
(VM4D-VM3D-VM2D-VM1D)
--------------------------------
      FUNCTION FUN3 ( TOL, R0, ERRE )
C
C
      COMMON / PASS / TAU
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```
      COMMON / RRRR / RRRR
      COMMON / NP / NP
      COMMON / PARAM / R, D, B, BZ, UMU
      COMMON / INTPAR / DEN, SR, SB, SBZ, SMU, RS0
      EXTERNAL FUN2
C
C
C     UNITS: (A) = MOLE/CC/SEC     (B) = 1/CM
C
C            4*PI*D*RHO(R0) = SOURCE TERM = A*EXP(-B*R0)
C
C
C     INTEGRAL OVER R0 FROM 0 TO INFINITY = SUM OF INTEGRAL FROM 0 TO RRRR
C     PLUS INTEGRAL FROM RRRR TO INFINITY.  IN LATTER INTEGRAL TRANSFORM FR
C     R0 TO S0 = RRRR**2/R0.  THIS INTEGRAL = INTEGRAL FROM 0 TO RRRR OF
C     RRRR**2/R0**2*F(RRRR**2/R0), OR IN TERMS OF S0 , S0/R0*F(S0).
C
C     GUARD AGAINST UNDERFLOW OF EXPONENTIAL ARGUMENT AT R0 = 0
C
      DEN = 4.E0*D*TAU
      SR = R
      SB = B
      SBZ = BZ
      SMU = UMU
C
C
      RS0 = R0
      XINT = VM2D(TOL,-1.,1.,FUN2,ERRE,0,9,NP)
      TERM1 = R0*R0*XINT
      ERRE1 = R0*R0*ERRE
C
      TERM2 = 0.E0
      ERRE2 = 0.
      IF( R0 .EQ. 0.E0) GO TO 10
      S0 = RRRR*RRRR/R0
      RS0 = S0
      XINT = VM2D(TOL,-1.,1.,FUN2,ERRE,0,9,NP)
C     TERM2 = (S0/R0) *  S0*S0  *   XINT
      TERM2 = S0*S0*S0/R0*XINT
      ERRE2 = S0*S0*S0/R0*ERRE
   10 CONTINUE
      FUN3 = (TERM1 + TERM2)
      ERRE = ERRE1 + ERRE2
      RETURN
      END
      FUNCTION FUN2(TOL, XMU0, ERRE)
      COMMON / INTPAR / DEN, R, B, BZ, MU, RS0
      REAL*4 MU0, MU
      PI = 3.14159265
C
```

```
      MU0 = XMU0
      Q = RS0
C
      ELLIP = 1. - 1./BZ/BZ
C
      SQ1 = SQRT(1. - ELLIP*MU0*MU0)
      SQ2 = SQRT((1. - MU*MU)*(1. - MU0*MU0))
C
C
      ARG = B*Q*SQ1 + (R*R - 2.*R*Q*(MU*MU0 + SQ2) + Q*Q)/DEN
      BARG = 2.*R*Q*SQ2/DEN
C
C   BESSL = EXP(-BARG)*I0(BARG)
C
      FUN2 = EXP(-ARG)*BESSL(BARG)
C
      ERRE = 1.E-7*FUN2
      RETURN
      END
      FUNCTION BESSL(X)
C
C   POLYNOMIAL APPROXIMATION TO EXP(-X)*I0(X) FROM
C   ABRAMOWITZ & STEGUN
C
      ABSX = ABS(X)
      T = ABSX/3.75
C
      IF(T .GT. 1.) GO TO 10
      S = T*T
      AI0 = 1. + 3.5156229*S + 3.0899424*S*S + 1.2067492*S**3 +
     $   .2659732*S**4 + .0360768*S**5 + .0045813*S**6
C
      BESSL = AI0*EXP(-ABSX)
      GO TO 20
   10 CONTINUE
      U = 1./T
      BESSL = .39894228 + .01328592*U + .00225319*U*U -
     1  .0157565*U**3 + .00916281*U**4 - .02057706*U**5
     2  + .02635537*U**6 - .01647633*U**7 + .00392377*U**8
C
      BESSL = BESSL/SQRT(ABSX)
   20 CONTINUE
C
      RETURN
      END
      FUNCTION VM4D(TOL,B,E,FUN2,ERRE,NW2,NM2,NMAXI)
      DIMENSION F(257), X(257),DE(257),ERR(257),AI(257)
C  THIS ROUTINE USES THE FIRST NM2 /2 POINTS IN AN EVENLY SPACED MESH
C THE ROUTINE USES AT MOST NMAX INTERVALS  RETURNING OR IF NW2=0, BEFORE
C BEFORE STOPPING
```

```
      NMAX=MINO(NMAXI,256)
      VM4D=0.
      ERRE=0.
      IF(E.EQ.B)RETURN
      TOL1=ABS(.5*TOL /(E-B))
C IN THIS VERSION THE FIRST FOUR POINTS HAVE AN UNUSUALLY LARGE
C TOLERANCE AND SERVE MAINLY TO LOCATE THE INPORTANT REGION
      TM=TOL1*200
      TC=TM
      NI=NM2 /2-1
      NI=MAXO(NI,3)
      AINC=(E-B) /NI
      NU=NI+1
      DO 3 I=1,NU
      X(I)=B+AINC*(I-1)
3     F(I)=FUN2(TM,X(I),ERR(I))
      DO 5 I=1,NI
5     AI(I)=ASINT(X,F,I,NI,ERR,DE(I))
      DE(NU)=0.
      AI(NU)=0.
20    ERRE=0.
      ERRS=0.
      VM4D=0.
      ERT=0.
      DO 30 I=1,NI
      ERT=ERT+.5*(ERR(I)+ERR(I+1))*(X(I+1)-X(I))
      VM4D=VM4D+AI(I)
      ERRS=ERRS+DE(I)*DE(I)
30    ERRE=ERRE+DE(I)
      ERRE=AMAX1(SQRT(ERRS),ABS(ERRE))
      IF(NW2.EQ.2)WRITE(6,116)NI,VM4D,ERRE
      IF(NI+1.LT.NM2)GOTO 100
      IF(ERRE.GT.TOL.AND.NI.LT.NMAX)GOTO100
116   FORMAT(' TEST',I5,E20.6,' +-',E10.3)
      NP=NI+1
      IF(NW2.EQ.0)RETURN
      IF(NW2.EQ.1.OR.NW2.EQ.4.)WRITE(6,103)(X(I),F(I),AI(I),DE(I),ERR
     * (I),I=1,NI)
      IF(NW2.EQ.1.OR.NW2.EQ.4.)WRITE(6,104)X(NP),F(NP),ERR(NP),NI
103   FORMAT(19X,'X',19X,'F',18X,'AI',18X,'DE',17X,'ERR' /(5E20.6))
104   FORMAT(2E20.6,40X,E20.6,' NI=',I5)
      WRITE(6,105)VM4D,ERRE,TOL
      IF(ERRE.LT.TOL)RETURN
      IF(NW2.EQ.3.OR.NW2.EQ.4)RETURN
105   FORMAT(' VM4D IS',E20.6,' +-',2E10.3,' NEED MORE POINTS TO DO',
     * 'BETTER')
      STOP
C  FINDING THE INTERVAL WITH THE LARGEST ERROR
100   CALL LERR(ICP,X,DE,AI,F,ERR,NI)
C RECALCULATING THE POINTS EFFECTED BY THE INSERTION OF X(ICP)
```

```
      DELT=X(ICP+1)-X(ICP-1)
      ERT=ERT-.5*(ERR(ICP-1)+ERR(ICP+1))*DELT
      TOL2=(.5*TOL-ERT) /DELT
      TC=TC /2.
      IF(TC.LT.TOL1)TC=0.
      TOL2=AMAX1(TOL2,TOL1,TC)
      IF(NW2.EQ.4)WRITE(6,102)NI,TOL2,TOL1,TOL
102   FORMAT(' TOL2 CHECK',I5,3E15.6)
      F(ICP)=FUN2(TOL2,X(ICP),ERR(ICP))
C  THE NEW POINT EFFECTS REGION BELOW, ITS OWN2, AND ONE ABOVE
      IF(ICP.GE.3)AI(ICP-2)=ASINT(X,F,ICP-2,NI,ERR,DE(ICP-2))
      AI(ICP-1)=ASINT(X,F,ICP-1,NI,ERR,DE(ICP-1))
      AI(ICP)=ASINT(X,F,ICP,NI,ERR,DE(ICP))
      IF(ICP.LT.NI)AI(ICP+1)=ASINT(X,F,ICP+1,NI,ERR,DE(ICP+1))
      GOTO20
      END
      FUNCTION VM3D(TOL,B,E,FUN2,ERRE,NW2,NM2,NMAXI)
      DIMENSION F(257), X(257),DE(257),ERR(257),AI(257)
C  THIS ROUTINE USES THE FIRST NM2 /2 POINTS IN AN EVENLY SPACED MESH
C THE ROUTINE USES AT MOST NMAX INTERVALS  RETURNING OR IF NW2=0, BEFORE
C BEFORE STOPPING
      NMAX=MIN0(NMAXI,256)
      VM3D=0.
      ERRE=0.
      IF(E.EQ.B)RETURN
      TOL1=ABS(.5*TOL /(E-B))
C IN THIS VERSION THE FIRST FOUR POINTS HAVE AN UNUSUALLY LARGE
C TOLERANCE AND SERVE MAINLY TO LOCATE THE IMPORTANT REGION
      TM=TOL1*200
      TC=TM
      NI=NM2 /2-1
      NI=MAX0(NI,3)
      AINC=(E-B) /NI
      NU=NI+1
      DO 3 I=1,NU
      X(I)=B+AINC*(I-1)
3     F(I)=FUN2(TM,X(I),ERR(I))
      DO 5 I=1,NI
5     AI(I)=ASINT(X,F,I,NI,ERR,DE(I))
      DE(NU)=0.
      AI(NU)=0.
20    ERRE=0.
      ERRS=0.
      VM3D=0.
      ERT=0.
      DO 30 I=1,NI
      ERT=ERT+.5*(ERR(I)+ERR(I+1))*(X(I+1)-X(I))
      VM3D=VM3D+AI(I)
      ERRS=ERRS+DE(I)*DE(I)
30    ERRE=ERRE+DE(I)
```

```
      ERRE=AMAX1(SQRT(ERRS),ABS(ERRE))
      IF(NW2.EQ.2)WRITE(6,116)NI,VM3D,ERRE
      IF(NI+1.LT.NM2)GOTO 100
      IF(ERRE.GT.TOL.AND.NI.LT.NMAX)GOTO100
116   FORMAT(' TEST',I5,E20.6,' +-',E10.3)
      NP=NI+1
      IF(NW2.EQ.0)RETURN
      IF(NW2.EQ.1.OR.NW2.EQ.4.)WRITE(6,103)(X(I),F(I),AI(I),DE(I),ERR
     * (I),I=1,NI)
      IF(NW2.EQ.1.OR.NW2.EQ.4.)WRITE(6,104)X(NP),F(NP),ERR(NP),NI
103   FORMAT(19X,'X',19X,'F',18X,'AI',18X,'DE',17X,'ERR' /(5E20.6))
104   FORMAT(2E20.6,40X,E20.6,' NI=',I5)
      WRITE(6,105)VM3D,ERRE,TOL
      IF(ERRE.LT.TOL)RETURN
      IF(NW2.EQ.3.OR.NW2.EQ.4)RETURN
105   FORMAT(' VM3D IS',E20.6,' +-',2E10.3,' NEED MORE POINTS TO DO',
     * 'BETTER')
      STOP
C  FINDING THE INTERVAL WITH THE LARGEST ERROR
100   CALL LERR(ICP,X,DE,AI,F,ERR,NI)
C RECALCULATING THE POINTS EFFECTED BY THE INSERTION OF X(ICP)
      DELT=X(ICP+1)-X(ICP-1)
      ERT=ERT-.5*(ERR(ICP-1)+ERR(ICP+1))*DELT
      TOL2=(.5*TOL-ERT) /DELT
      TC=TC /2.
      IF(TC.LT.TOL1)TC=0.
      TOL2=AMAX1(TOL2,TOL1,TC)
      IF(NW2.EQ.4)WRITE(6,102)NI,TOL2,TOL1,TOL
102   FORMAT(' TOL2 CHECK',I5,3E15.6)
      F(ICP)=FUN2(TOL2,X(ICP),ERR(ICP))
C   THE NEW POINT EFFECTS REGION BELOW, ITS OWN2, AND ONE ABOVE
      IF(ICP.GE.3)AI(ICP-2)=ASINT(X,F,ICP-2,NI,ERR,DE(ICP-2))
      AI(ICP-1)=ASINT(X,F,ICP-1,NI,ERR,DE(ICP-1))
      AI(ICP)=ASINT(X,F,ICP,NI,ERR,DE(ICP))
      IF(ICP.LT.NI)AI(ICP+1)=ASINT(X,F,ICP+1,NI,ERR,DE(ICP+1))
      GOTO20
      END
      FUNCTION VM2D(TOL,B,E,FUN2,ERRE,NW2,NM2,NMAXI)
      DIMENSION F(257),  X(257),DE(257),ERR(257),AI(257)
C   THIS ROUTINE USES THE FIRST NM2 /2 POINTS IN AN EVENLY SPACED MESH
C THE ROUTINE USES AT MOST NMAX INTERVALS  RETURNING OR IF NW2=0, BEFORE
C BEFORE STOPPING
      NMAX=MIN0(NMAXI,256)
      VM2D=0.
      ERRE=0.
      IF(E.EQ.B)RETURN
      TOL1=ABS(.5*TOL /(E-B))
C IN THIS VERSION THE FIRST FOUR POINTS HAVE AN UNUSUALLY LARGE
C TOLERANCE AND SERVE MAINLY TO LOCATE THE IMPORTANT REGION
      TM=TOL1*200
```

```
      TC=TM
      NI=NM2 /2-1
      NI=MAX0(NI,3)
      AINC=(E-B) /NI
      NU=NI+1
      DO 3 I=1,NU
      X(I)=B+AINC*(I-1)
3     F(I)=FUN2(TM,X(I),ERR(I))
      DO 5 I=1,NI
5     AI(I)=ASINT(X,F,I,NI,ERR,DE(I))
      DE(NU)=0.
      AI(NU)=0.
20    ERRE=0.
      ERRS=0.
      VM2D=0.
      ERT=0.
      DO 30 I=1,NI
      ERT=ERT+.5*(ERR(I)+ERR(I+1))*(X(I+1)-X(I))
      VM2D=VM2D+AI(I)
      ERRS=ERRS+DE(I)*DE(I)
30    ERRE=ERRE+DE(I)
      ERRE=AMAX1(SQRT(ERRS),ABS(ERRE))
      IF(NW2.EQ.2)WRITE(6,116)NI,VM2D,ERRE
      IF(NI+1.LT.NM2)GOTO 100
      IF(ERRE.GT.TOL.AND.NI.LT.NMAX)GOTO100
116   FORMAT(' TEST',I5,E20.6,' +-',E10.3)
      NP=NI+1
      IF(NW2.EQ.0)RETURN
      IF(NW2.EQ.1.OR.NW2.EQ.4.)WRITE(6,103)(X(I),F(I),AI(I),DE(I),ERR
     * (I),I=1,NI)
      IF(NW2.EQ.1.OR.NW2.EQ.4.)WRITE(6,104)X(NP),F(NP),ERR(NP),NI
103   FORMAT(19X,'X',19X,'F',18X,'AI',18X,'DE',17X,'ERR' /(5E20.6))
104   FORMAT(2E20.6,40X,E20.6,' NI=',I5)
      WRITE(6,105)VM2D,ERRE,TOL
      IF(ERRE.LT.TOL)RETURN
      IF(NW2.EQ.3.OR.NW2.EQ.4)RETURN
105   FORMAT(' VM2D IS',E20.6,' +-',2E10.3,' NEED MORE POINTS TO DO',
     * 'BETTER')
      STOP
C  FINDING THE INTERVAL WITH THE LARGEST ERROR
100   CALL LERR(ICP,X,DE,AI,F,ERR,NI)
C RECALCULATING THE POINTS EFFECTED BY THE INSERTION OF X(ICP)
      DELT=X(ICP+1)-X(ICP-1)
      ERT=ERT-.5*(ERR(ICP-1)+ERR(ICP+1))*DELT
      TOL2=(.5*TOL-ERT) /DELT
      TC=TC /2.
      IF(TC.LT.TOL1)TC=0.
      TOL2=AMAX1(TOL2,TOL1,TC)
      IF(NW2.EQ.4)WRITE(6,102)NI,TOL2,TOL1,TOL
102   FORMAT(' TOL2 CHECK',I5,3E15.6)
```

```
      F(ICP)=FUN2(TOL2,X(ICP),ERR(ICP))
C   THE NEW POINT EFFECTS REGION BELOW. ITS OWN2, AND ONE ABOVE
      IF(ICP.GE.3)AI(ICP-2)=ASINT(X,F,ICP-2,NI,ERR,DE(ICP-2))
      AI(ICP-1)=ASINT(X,F,ICP-1,NI,ERR,DE(ICP-1))
      AI(ICP)=ASINT(X,F,ICP,NI,ERR,DE(ICP))
      IF(ICP.LT.NI)AI(ICP+1)=ASINT(X,F,ICP+1,NI,ERR,DE(ICP+1))
      GOTO20
      END
      FUNCTION VM1D(TOL,B,E,FUN2,ERRE,NW2,NM2,NMAXI)
      DIMENSION F(257), X(257),DE(257),ERR(257),AI(257)
C NOTE THAT NW2=0 IMPLIES NO INTERNAL OUTPUT AND WILL ALWAYS RETURN
C NW2=1 IMPLIES A WRITE OUT OF ALL INTERMEDIATE VALUES AND WILL STOP
C IF IT IS NOT POSSIBLE TO REACH THE DESIRED TOLERANC
C NW2=2 WILL WRITE ALL INTERMEDIATE INTEGRATION VALUES AND WILL STOP
C IF DESIRED TOL NOT REACHED. NW2=3 WILL WRITE OUT FINAL INTEGRATION
C RESULT AND WILL ALWAYS RETURN. NW2=4 WILL WRITE OUT INTERMEDIATE
C VALUES AND WILL ALWAYS RETURN.
C  THIS ROUTINE USES THE FIRST NM2 /2 POINTS IN AN EVENLY SPACED MESH
C THE ROUTINE USES AT MOST NMAX INTERVALS  RETURNING OR IF NW2=0, BEFORE
C BEFORE STOPPING
      NMAX=MIN0(NMAXI,256)
      VM1D=0.
      ERRE=0.
      IF(E.EQ.B)RETURN
      TOL1=ABS(.5*TOL /(E-B))
C IN THIS VERSION THE FIRST FOUR POINTS HAVE AN UNUSUALLY LARGE
C TOLERANCE AND SERVE MAINLY TO LOCATE THE IMPORTANT REGION
      TM=TOL1*200
      TC=TM
      NI=NM2 /2-1
      NI=MAX0(NI,3)
      AINC=(E-B) /NI
      NU=NI+1
      DO 3 I=1,NU
      X(I)=B+AINC*(I-1)
3     F(I)=FUN2(TM,X(I),ERR(I))
      DO 5 I=1,NI
5     AI(I)=ASINT(X,F,I,NI,ERR,DE(I))
      DE(NU)=0.
      AI(NU)=0.
20    ERRE=0.
      ERRS=0.
      VM1D=0.
      ERT=0.
      DO 30 I=1,NI
      ERT=ERT+.5*(ERR(I)+ERR(I+1))*(X(I+1)-X(I))
      VM1D=VM1D+AI(I)
      ERRS=ERRS+DE(I)*DE(I)
30    ERRE=ERRE+DE(I)
      ERRE=AMAX1(SQRT(ERRS),ABS(ERRE))
```

```
      IF(NW2.EQ.2)WRITE(6,116)NI,VM1D,ERRE
      IF(NI+1.LT.NM2)GOTO 100
      IF(ERRE.GT.TOL.AND.NI.LT.NMAXI)GOTO100
116   FORMAT(' TEST',I5,E20.6,' +-',E10.3)
      NP=NI+1
      IF(NW2.EQ.0)RETURN
      IF(NW2.EQ.1.OR.NW2.EQ.4.)WRITE(6,103)(X(I),F(I),AI(I),DE(I),ERR
     * (I),I=1,NI)
      IF(NW2.EQ.1.OR.NW2.EQ.4.)WRITE(6,104)X(NP),F(NP),ERR(NP),NI
103   FORMAT(19X,'X',19X,'F',18X,'AI',18X,'DE',17X,'ERR' /(5E20.6))
104   FORMAT(2E20.6,40X,E20.6,' NI=',I5)
      WRITE(6,105)VM1D,ERRE,TOL
      IF(ERRE.LT.TOL)RETURN
      IF(NW2.EQ.3.OR.NW2.EQ.4)RETURN
105   FORMAT(' VM1D IS',E20.6,' +-',2E10.3,' NEED MORE POINTS TO DO',
     * 'BETTER')
      STOP
C  FINDING THE INTERVAL WITH THE LARGEST ERROR
100   CALL LERR(ICP,X,DE,AI,F,ERR,NI)
C RECALCULATING THE POINTS EFFECTED BY THE INSERTION OF X(ICP)
      DELT=X(ICP+1)-X(ICP-1)
      ERT=ERT-.5*(ERR(ICP-1)+ERR(ICP+1))*DELT
      TOL2=(.5*TOL-ERT) /DELT
      TC=TC /2.
      IF(TC.LT.TOL1)TC=0.
      TOL2=AMAX1(TOL2,TOL1,TC)
      IF(NW2.EQ.4)WRITE(6,102)NI,TOL2,TOL1,TOL
102   FORMAT(' TOL2 CHECK',I5,3E15.6)
      F(ICP)=FUN2(TOL2,X(ICP),ERR(ICP))
C   THE NEW POINT EFFECTS REGION BELOW, ITS OWN2, AND ONE ABOVE
      IF(ICP.GE.3)AI(ICP-2)=ASINT(X,F,ICP-2,NI,ERR,DE(ICP-2))
      AI(ICP-1)=ASINT(X,F,ICP-1,NI,ERR,DE(ICP-1))
      AI(ICP)=ASINT(X,F,ICP,NI,ERR,DE(ICP))
      IF(ICP.LT.NI)AI(ICP+1)=ASINT(X,F,ICP+1,NI,ERR,DE(ICP+1))
      GOTO20
      END
      SUBROUTINE LERR(ICP,X,DE,AI,F,ERR,NI)
      DIMENSION X(257),DE(257),AI(257),F(257),ERR(257)
      DC=ABS(DE(1))
C FINDING THE INTERVAL WITH THE LARGEST ERROR ESTIMATE
      IC=1
      DO 110 I=2,NI
      IF(DC.GT.ABS(DE(I)))GOTO110
      DC=ABS(DE(I))
      IC=I
110   CONTINUE
C   MOVING THE STACK
      ICP=IC+1
      NI=NI+1
      NBP=NI+ICP+1
```

```
      NB=NI+ICP
      DO 120 I=ICP,NI
      ERR(NBP-I)=ERR(NB-I)
      AI(NBP-I)=AI(NB-I)
      X(NBP-I)=X(NB-I)
      F(NBP-I)=F(NB-I)
120   DE(NBP-I)=DE(NB-I)
C INSERTING THE NEW POINT WHICH WILL BE USED BY THE MAIN ROUTINE
      X(ICP)=.5*(X(IC)+X(IC+2))
      RETURN
      END
      FUNCTION ASINT(X,F,I,NI,ERR,DE)
C ROUTINE CALCULATES THE INTEGRAL ESTIMATE BETWEEN X(I) AND X(I+1) USING
C BEST FIT TO NEARBY FOUR POINTS AND THE ERROR IN THIS ESTIMATE BY SUMMI
C THE SQUARES OF THE DIFFERENCES CAUSED BY USING FITS WHICH SUCCESSIVELY
C OUT EACH OF THE POSSIBLE FOUR FITS + THE SQUARE OF THE AVERAGE ERROR I
C FUNCTION TIMES THE INTERVAL.
      DIMENSION X(257),F(257),ERR(257),A0(5),A2(5)
      IB=I
      IF(IB.EQ.1) IB=2
      IF(I.EQ.NI)IB=NI-1
      X0=.5*(X(I)+X(I+1))
      CALL FITS(X0,X,F,IB,A0,A2)
      C1=X(I+1)-X(I)
      C3=C1**3 /12.
      ASINT=A0(1)*C1+A2(1)*C3
      ERRS=0.
      DO 10 J=2,5
      AWP=A0(J)*C1+A2(J)*C3
      IF(ASINT.EQ.AWP)GOTO10
      ADIFF=ABS(ASINT-AWP)
      IF(ADIFF.LT.1.E-12)GOTO10
      ERRS=ERRS+ADIFF**2
10    CONTINUE
      DE=ERRS+(.5*(ERR(I)+ERR(I+1))*C1)**2
      DE=SIGN(SQRT(DE),ASINT-AWP)
      RETURN
      END
-------------------------------
              CYL3
COMMENT:  CONTINUATION OF CYL2
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      SUBROUTINE FITS(X0,X,F,IB,A0,A2)
C ROUTINE DOES A FIT OF FORM A0+A1*X+A2*X**2 TO FOUR POINTS.  X IS MEASU
C THE CENTER OF THE INTERVAL OF INTEREST SO A1 IS NOT NEEDED TO DO INTEG
C AND HENCE IS NOT CALCULATED.  THE FITTED CONSTANTS ARE IN A0(1) AND A2
C A0(2-5) AND A2(2-5) CONTAINCNSTANTS FOR THE FITS RESULTING FROM LEAVIN
C EACH OF THE POSSIBLE POINTS IN TURN.
      DIMENSION X(257),F(257),A0(5),A2(5)
      EPP=1.E-5
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```
      ETA=1.E-3
      FF0=0.
      FF1=0.
      FF2=0.
      S0=4.
      S1=0.
      S2=0.
      S3=0.
      S4=0.
      DO 20 J=1,4
      FS=F(IB+J-2)
      XD=X(IB+J-2)-X0
      FF0=FF0+FS
      FF1=FF1+FS*XD
      S1=S1+XD
      XP=XD*XD
      FF2=FF2+FS*XP
      S2=S2+XP
      XP=XP*XD
      S3=S3+XP
      XP=XP*XD
      S4=S4+XP
20    CONTINUE
      IC=1
30    CM=1. /(S2+EPP)
      FC1=FF2-CM*S3*FF1
      FC2=FF0-CM*S1*FF1
      SC1=S2-CM*S1*S3
      SC2=S4+ETA-CM*S3*S3
      SC3=S0-CM*S1*S1
      IF(ABS(SC2).LT.1.E-7)SC2=SIGN(1.E-7,SC2)
      A0(IC)=(FC2-FC1*SC1 /SC2)/(SC3-SC1**2/SC2)
      A2(IC)=(FC1-A0(IC)*SC1) /SC2
      IF(IC.EQ.5)RETURN
      S0=3.
      FS=F(IB+IC-2)
      FA=0.
      IF(IC.GT.1)FA=F(IB+IC-3)
      XS=X(IB+IC-2)-X0
      XA=0.
      IF(IC.GT.1)XA=X(IB+IC-3)-X0
      FF0=FF0+FA-FS
      S1=S1+XA-XS
      FF1=FF1+XA*FA-XS*FS
      XPA=XA*XA
      XPS=XS*XS
      FF2=FF2+XPA*FA-XPS*FS
      S2=S2+XPA-XPS
      XPA=XA*XPA
      XPS=XPS*XS
```

```
      S3=S3+XPA-XPS
      XPA=XA*XPA
      XPS=XPS*XS
      S4=S4+XPA-XPS
      IC=IC+1
      GOTO30
      END
-------------------------------
*******************************
-------------------------------
                AXII
COMMENT:  THIS CALLS VM2D-VM1D
-------------------------------
C  THIS PROGRAM CALCU_ATES THE STEADY STATE SOLUTION TO THE DIFFUSION
C  EQUATION IN AXISYMMETRIC GEOMETRY FOR STEADY STATE SOURCE -- I.E. THE
C  AXISYMMETRIC POISSON EQUATION
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 MU, MUX
      DIMENSION RPX(15), MUX(37), C(15,37), THX(37), PL(10,37)
      DIMENSION VL(10,15), EL(10,15), E(15,37), CL(15,37)
      DIMENSION EPL(15,37), RX(15)
      COMMON   ECC, RP, L, NP, NPX2
      EXTERNAL FUN2F, FUN2G
C
      DATA PI/ 3.141592653589793 /
C
      READ(5,*) A, D, B, BZ, LMX
C  LMX SHOULD BE EVEN BECAUSE ONLY EVEN TERMS CONTRIBUTE
      ECC = DSQRT(1.D0 - 1.D0/BZ/BZ)
      JX = LMX + 1
      NP = 9
      READ(5,*) NPX,ANPX2,BNPX2
      WRITE(6,*) A, D, B, BZ, ECC, LMX
      WRITE(6,*) NP, NPX
C
C
      READ(5,*) MUSKIP,  IHALF
C  MUSKIP MUST EQUAL AN INTEGER DIVISOR OF 36
C  IF IHALF=1 ONLY GO FROM 0 TO 90 DEG. IF IHALF = 0 GO FORM 0 TO 180 DE
C
      MUTOP = 1 + 18*(2 - IHALF)
C
      DO 10 I = 1, MUTOP, MUSKIP
      THX(I) = 5.D0*(I-1)
      MUX(I) = DCOS(THX(I)*PI/180.D0)
      MU = MUX(I)
C
C  CALCULATE LEGENDRE POLYNOMIALS AT MU
C
```

```
      PL(1,I) = 1.D0
      PL(2,I) = MU
C
      IF(JX .LE. 2) GO TO 15
      DO 11 J = 3,JX
   11 PL(J,I) = ((2.D0*J-3.D0)*MU*PL(J-1,I) - (J-2.D0)*PL(J-2,I))/
     $  (J-1)
   15 CONTINUE
   10 CONTINUE
C
C  ASSIGN RPX(I)
C
      READ(5,*) IX,ISKIP
      CALL CLOSE(5)
      WRITE(6,*) IX,ISKIP
      DATA RPX/ .1D0, .5D0, 1.D0, 1.5D0, 2.D0, 3.D0, 4.D0, 6.D0,
     1  10.D0, 15.D0, 20.D0, 30.D0, 3*40.D0 /
C  RPX CANNOT BE ZERO.
C
C
C  LOOP OVER R AND MU TO CALCULATE GRID OF SOLUTION VALUES
C
      DO 100 I = 1, IX, ISKIP
      RP = RPX(I)
      DO 95 J=1, JX, 2
C
      L = J - 1
      FL = RP**L
      GL = RP**(-L-1)
C
      NPX2 = 2**(ANPX2 + L/BNPX2)
      IF(NPX2 .GT. 256) NPX2 = 256
C
      TOL = 0.D0
      FCOEF = VM2D(TOL,0.D0,RP,FUN2F,ERRE,0,NP,NPX)
      ERREF = ERRE
      VLF = FCOEF*FL
      ELF = ERREF*FL
C
      TOL = 0.D0
      GCOEF = VM2D(TOL,0.D0,RP,FUN2G,ERRE,0,NP,NPX)
      ERREG = ERRE
      VLG = GCOEF*GL
      ELG = ERREG*GL
C
C
      VL(J,I) = VLF + VLG
      EL(J,I) = ELF + ELG
C
C  WRITE OUT INTERMEDIATE QUANTITIES
```

⋮

```
      WRITE(6,345) L,RP,FL,GL,FCOEF,GCOEF,VLF,VLG,VL(J,I)
      WRITE(6,346)                ERREF,ERREG,ELF,ELG,EL(J,I)
   95 CONTINUE
C
      WRITE(6,347)
      DO 90 K = 1, MUTOP, MUSKIP
C  UNCONVENTIONAL NESTING ORDER I-K-J TO PRESERVE J AS THE PARTIAL WAVE
C  INDEX
      TH = THX(K)
      MU = MUX(K)
      WRITE(6,103) RP,TH,MU
C
      C(I,K) = 0.D0
      E(I,K) = 0.D0
      DO 85 J=1, JX, 2
      L = J - 1
      CL(I,K) = VL(J,I)*PL(J,K)
      EPL(I,K) = EL(J,I)*PL(J,K)
C
      RELERR = 0.D0
      IF(CL(I,K) .EQ. 0.D0) GO TO 1199
      RELERR = EPL(I,K)/CL(I,K)
 1199 CONTINUE
C
      C(I,K) = C(I,K) + CL(I,K)
      E(I,K) = E(I,K) + EPL(I,K)
      WRITE(6,104) L,C(I,K),E(I,K),CL(I,K),EPL(I,K),RELERR
   85 CONTINUE
C
C
   90 CONTINUE
  100 CONTINUE
C
  103 FORMAT(1H0,D12.5,1X,F8.3,2X,1PD12.5/)
  104 FORMAT(1H ,T3,I2,5X,2(1PD12.5,1X,D12.5,5X),(3(1PD12.5,1X,
     @    D12.5)))
  345 FORMAT(1H0,I2,1P8E12.4)
  346 FORMAT(1H ,38X,1P5E12.4)
  347 FORMAT(1H0///)
      STOP
      END
      FUNCTION FUN2F(TOL, SHOP, ERRE)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 JACOBI
      COMMON    ECC, RP, L, NP, NPX2
      COMMON /SEND/ RHOPP
      EXTERNAL FUN1
C
C
      FUN2F = 0.D0
```

```
      ERRE = 0.D0
      IF(SHOP .LE. 1.D-14) GO TO 100
      RHOP = RP*RP/SHOP
        RHOPP = RHOP
      VARPM = RHOP**(1-L)
      JACOBI = RP*RP/SHOP/SHOP
      XINT = VM1D(TOL,0.D0,1.D0,FUN1,ERRE,0,NP,NPX2)
      ERRE = ERRE
      FUN2F = VARPM*JACOBI*XINT
      ERRE = VARPM*JACOBI*ERRE
C  FACTORS OF (2*L+1) IN DENOM. OF VARPM AND NUM. OF XINT CANCEL
C  AND ARE THEREFORE EXTRACTED.  FACTOR OF 0.5 IN XINT REMAINS, EXTRACTE
C  THEN MULTIPLIED BY FACTOR OF 2. FROM TAKING INTEGRAL OF EVEN INTEGRAN
C  OVER HALF THE RANGE GIVES A FINAL FACTOR OF 1.
  100 CONTINUE
C     WRITE(6,333) L,RHOP,XINT,VARPM,FUN2F
  333 FORMAT(1H ,I2,2X,1PE12.4)
      RETURN
      END
      FUNCTION FUN2G(TOL, RHOP, ERRE)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /SEND/ RHOPP
      COMMON   ECC, RP, L, NP, NPX2
      EXTERNAL FUN1
C
C
      RHOPP = RHOP
      VARPM = RHOP**(L+2)
      XINT = VM1D(TOL,0.D0,1.D0,FUN1,ERRE,0,NP,NPX2)
      ERRE = ERRE
      FUN2G = VARPM*XINT
      ERRE = VARPM*ERRE
C  FACTORS OF (2*L+1) IN DENOM. OF VARPM AND NUM. OF XINT CANCEL
C  AND ARE THEREFORE EXTRACTED.  FACTOR OF 0.5 IN XINT REMAINS, EXTRACTE
C  THEN MULTIPLIED BY FACTOR OF 2. FROM TAKING INTEGRAL OF EVEN INTEGRAN
C  OVER HALF THE RANGE GIVES A FINAL FACTOR OF 1.
  100 CONTINUE
C     WRITE(6,333) L,SHOP,RHOP,XINT,VARPM,JACOBI,FUN2G
  333 FORMAT(1H ,I2,2X,1PE12.4)
      RETURN
      END
      FUNCTION FUN1(TOL, X, ERRE)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON   ECC, RP, L, NP, NPX2
      COMMON /SEND/ RHOP
      DIMENSION PL(10)
      FUN1 = DEXP(-RHOP*DSQRT(1. - (ECC*X)**2))
C-----------------------------------------------------------------
      PL(1) = 1.D0
      PL(2) = X
```

```
C
      JJ = L + 1
      IF(JJ .LE. 2) GO TO 15
      DO 11 J = 3,JJ
   11 PL(J) = ((2.D0*J-3.D0)*X*PL(J-1) - (J-2.D0)*PL(J-2))/(J-1)
   15 CONTINUE
C-----------------------------------------------------------------
      FUN1 = FUN1*PL(JJ)
      ERRE = 1.D-14*FUN1
      RETURN
      END
C     EXTERNAL FUN2
C     ANAL=1.6181900/2.D0
C     B=0.
C     E=DSQRT(15.)
C     TOL=2.
C     DO 10 J=1,10
C     ANUM=VM2D(TOL,B,E,FUN2,ERRE,0,9,256)
C     WRITE(6,101)J,TOL,ANUM,ERRE,ANAL
C101  FORMAT(I5,2F10.7,' ←-',E10.3,F10.7)
C     TOL=.5*TOL
C10   CONTINUE
C     STOP
C     END
C     FUNCTION FUN1(TOL,X,ERRE)
C     IMPLICIT REAL*8 (A-H,O-Z)
C     COMMON/PASS/Y
C     FUN1=COS(X*Y)
C     ERRE=1.D-14
C     RETURN
C     END
C     FUNCTION FUN2(TOL,Y,ERRE)
C     IMPLICIT REAL*8 (A-H,O-Z)
C     EXTERNAL FUN1
C     COMMON/PASS/PY
C     PY=Y
C     B=0.
C     E=Y
C     FUN2=VM1D(TOL,B,E,FUN1,ERRE,0,9,256)
C     RETURN
C     END
-------------------------------
*******************************
-------------------------------
```

CHAPTER V

```
              KINRR
-----------------------------
@@KINRR JOB (2003,5006,5,10),PAUL,CLASS=2
@*PASSWORD
@*ROUTE PRINT LOCAL
@@ EXEC FORTXCG
C
C-----------------------------------------------------------------------
C  1. CHECK MASS BALANCE IN KINETIC PROGRAM
C  2. DISPLAY REACTION RATES AND PRODUCTION RATES
C
C-----------------------------------------------------------------------
C
      DIMENSION A(11,1), AH(1), AO(1), YI(12,1), RX(1)
      DIMENSION YH(1), YO(1), YTH(1), YTO(1)
C
      DIMENSION RRC(34), RR(34), PRC(8,34), ISTOI(8,34)
      DIMENSION IST(8,17), PR(8)
      DIMENSION AA(11)
      EQUIVALENCE (A(1),AA(1))
C
C  J = 1  H       POS. YIELD
C      2  H2      POS. YIELD
C      3  H2O     NEG. YIELD
C      4  HO2
C      5  H2O2
C      6  O       POS. YIELD
C      7  OH      POS. YIELD
C      8  O2
C
      CALL ERRSET(208,2000,-1,1)
C
C
C
C  HARDWIRED.  TEMPORARY.  400 K:
      DATA RRC/  1.24E05, 6.29E12, 9.95E07, 5.30E08,
     1 3.18E03, 7.91E11, 7.72E02, 3.35E10, 1.03E12, 3.43E-5,
     2 9.26E-42, 8.81E17, 5.83E15, 1.90E-10, 1.42E13, 7.54E-18,
     3 2.29E13, 1.47E-9, 1.04E13, 1.43E-18, 1.42E13, 2.76E-26,
     4 2.00E-10, 2.84E12, 1.65E-08, 5.38E17, 1.51E10, 43.84,
     5 1.00E16, 4.19E-40, 7.45E-48, 8.74E14, 7.66E-39, 3.02E15 /
C
C  HARDWIRED.  TEMPORARY.  300 K:  (REMEMBER TO COME IN HERE AND DO
C  MINOR SURGERY WHEN YOU WANT IT CHANGED TO THIS TEMPERATURE.  IF AND
C  WHEN YOU WANT ANY TEMPERATURE, MODIFY THIS.
C
C     DATA RRC/ 1.09E2, 4.73E12, 1.76E6, 2.16E7, 1.45, 5.00E11,
C    1 1.55E-1, 3.87E9, 4.88E11, 3.64E-11, 7.00E-60, 1.57E18,
C    2 8.88E15, 8.30E-19, 9.36E12, 3.68E-28, 1.04E13, 7.32E-17,
C    3 7.76E12, 4.26E-29, 9.36E12, 9.74E-40, 3.42E-18, 1.87E12,
```

```
C     4 8.52E-17, 4.51E18, 3.15E9, 1.72E-2, 1.00E16, 0., 0.,
C     5 9.47E14, 2.50E-56, 3.02E15 /
C
      DATA IST/ -1, 0, 0, 0, 0, 1, 1,-1,
     2           1,-1, 0, 0, 0,-1, 1, 0,
     3           0, 0,-1, 0, 0,-1, 2, 0,
     4          -1, 1,-1, 0, 0, 0, 1, 0,
     5           0, 0, 1,-1, 1, 0,-1, 0,
     6           1, 0,-1, 0, 0, 0, 1, 0,
     7          -1, 0, 0, 0, 1, 0, 0,-1,
     8           0, 0, 0, 0,-1,-1, 1, 1,
     9          -1, 0, 0, 0,-1, 0, 2, 0,
     X          -1, 1, 0, 0,-1, 0, 0, 1,
     1           0, 0, 1, 0,-1, 0,-1, 1,
     2           0, 0, 0,-1, 2, 0, 0,-1,
     3           0, 0, 0,-1, 0, 0, 2, 0,
     4          -1, 1, 0,-1, 1, 0, 0, 0,
     5          -1, 0, 0, 0, 0,-1, 1, 0,
     6           0, 0, 0, 0, 0, 2, 0,-1,
     7           2,-1, 0, 0, 0, 0, 0, 0/
C
C  CORRECT SWITCH OF H2O2 WITH HO2 (INADVERTENT)
C
      DO 1025 I = 1,17
      ISTSAV = IST(4,I)
      IST(4,I) = IST(5,I)
 1025 IST(5,I) = ISTSAV
C
C
C
      DO 25 K = 1,17
      DO 25 J = 1,8
      KE = 2*K
      KO = KE-1
      ISTOI(J,KO) = IST(J,K)
      ISTOI(J,KE) = -IST(J,K)
   25 CONTINUE
C
C
C
      NS = 8
C
C     AH2O = 0.99626E-08
C     XAH2O = 0.00001E-08
C
C-------------READ STARTING SECTION-----------------------------------------
C
C
      NSKIPM = 11
      DO 210 I = 1,NSKIPM
```

```
      READ(8,1) QAQ
  210 CONTINUE
    1 FORMAT(A4)
C
C
C   NOW READ YI(J,1)  (THE YIELDS)
      READ(8,3) RX(1),(YI(J,1),J=1,8)
    3 FORMAT(T7,1P9E11.4)
C
      NSKIPM = 8
      DO 310 I = 1,NSKIPM
      READ(8,1) QAQ
  310 CONTINUE
C
C-----------------------------------------------------------------------------
C   HERE START READ LOOP
C
      READ(5,*) IPAGE
      DO 1000 KK = 1,IPAGE
C
      NLOOP = 6
      DO 410 I = 1,NLOOP
      READ(8,1) QAQ
  410 CONTINUE
C   NOW READ X  (TIME)
      XSAV = X
      READ(8,4) X
    4 FORMAT(T5,E14.7)
C   NOW READ DX (IN CASE)
      DXSAV = DX
      READ(8,5) DX, NSTEP
    5 FORMAT(T7,E14.7,16X,I7)
C*****************************************          READ(8,1) QAQ
C   NOW READ A(J,1) (THE CONCENTRATIONS)
      READ(8,6) (A(J,1),J=1,8)
    6 FORMAT(T13,1P8E11.4)
C   6 FORMAT(T16,1P8E11.4)
C
      IF (KK .NE. 1) GO TO 252
      AH2O = A(3,1)
      XAH2O = .0001*AH2O
  252 CONTINUE
C
C
C END OF READ ---------------------------------------------------------------
C
C
      MPSI = 1
      DO 100 I = 1, MPSI
C
```

```
      YH(I) = YI(1,I) + 2.*YI(2,I) + YI(7,I)
      YTH(I) = YH(I) + 2.*YI(3,I)
C
      YO(I) = YI(6,I) + YI(7,I)
      YTO(I) = YO(I) + YI(3,I)
C
      YI(9,I) = YH(I)
      YI(10,I) = YTH(I)
      YI(11,I) = YO(I)
      YI(12,I) = YTO(I)
C
      A(11,I) = A(3,I) - AH20
C.......................      IF(A(11,I) .LT. XAH20) A(13,I) = 0.
C  BELOW THE LIMIT OF NUMERICAL ROUNDOFF ERROR
C
      AH(I) = A(1,I) + 2.*A(2,I) + 2.*0. + A(4,I) + 2.*A(5,I) +
     @  A(7,I)
      AO(I) = 0. + 2.*A(4,I) + 2.*A(5,I) + A(6,I) + A(7,I) +
     $  2.*A(8,I)
C
      A(9,I) = AH(I)
      A(10,I) = AO(I)
C
      WRITE(6,1999)
      WRITE(6,1501) (YI(J,I),J=1,12)
      WRITE(9,1501) (YI(J,I),J=1,12)
      WRITE(6,2002)
      WRITE(6,1501) (A(J,I),J=1,11)
      WRITE(9,1501) (A(J,I),J=1,11)
      WRITE(6,2002)
C
      RAT = 0.
      IF(AO(I) .EQ. 0.) GO TO 272
      RAT = AH(I)/AO(I)
      CORAT = RAT - 2.
  272 CONTINUE
C
      WRITE(6,1501) AH(I), AO(I), RAT, CORAT
      WRITE(9,1501) AH(I), AO(I), RAT, CORAT
      WRITE(6,2000)
  100 CONTINUE
C
C
C  CORRECT SWITCH OF H202 AND HO2 (INADVERTENT)
      AASAV = AA(4)
      AA(4) = AA(5)
      AA(5) = AASAV
C
      RR(1) = RRC(1)*AA(1)*AA(8)
      RR(2) = RRC(2)*AA(6)*AA(7)
```

```
      RR(3) = RRC(3)*AA(2)*AA(6)
      RR(4) = RRC(4)*AA(1)*AA(7)
      RR(5) = RRC(5)*AA(3)*AA(6)
      RR(6) = RRC(6)*AA(7)*AA(7)
      RR(7) = RRC(7)*AA(3)*AA(1)
      RR(8) = RRC(8)*AA(2)*AA(7)
      RR(9) = RRC(9)*AA(4)*AA(7)
      RR(10) = RRC(10)*AA(3)*AA(5)
      RR(11) = RRC(11)*AA(3)*AA(3)
      RR(12) = RRC(12)*AA(1)*AA(7)*AA(3)
      RR(13) = RRC(13)*AA(1)*AA(8)*AA(3)
      RR(14) = RRC(14)*AA(5)*AA(3)
      RR(15) = RRC(15)*AA(5)*AA(6)
      RR(16) = RRC(16)*AA(7)*AA(8)
      RR(17) = RRC(17)*AA(5)*AA(1)
      RR(18) = RRC(18)*AA(7)*AA(7)
      RR(19) = RRC(19)*AA(5)*AA(1)
      RR(20) = RRC(20)*AA(2)*AA(8)
      RR(21) = RRC(21)*AA(5)*AA(7)
      RR(22) = RRC(22)*AA(3)*AA(8)
      RR(23) = RRC(23)*AA(4)*AA(8)
      RR(24) = RRC(24)*AA(5)*AA(5)
      RR(25) = RRC(25)*AA(4)*AA(3)
      RR(26) = RRC(26)*AA(7)*AA(7)*AA(3)
      RR(27) = RRC(27)*AA(4)*AA(1)
      RR(28) = RRC(28)*AA(5)*AA(2)
      RR(29) = RRC(29)*AA(6)*AA(1)*AA(3)
      RR(30) = RRC(30)*AA(7)*AA(3)
      RR(31) = RRC(31)*AA(8)*AA(3)
      RR(32) = RRC(32)*AA(6)*AA(6)*AA(3)
      RR(33) = RRC(33)*AA(2)*AA(3)
      RR(34) = RRC(34)*AA(1)*AA(1)*AA(3)
C
C  SWITCH BACK
      AASAV = AA(4)
      AA(4) = AA(5)
      AA(5) = AASAV
C
C
C
      DO 30 J = 1, 8
      PR(J) = 0.
      DO 30 K = 1, 34
      PRC(J,K) = RR(K)*ISTOI(J,K)
      PR(J) = PR(J) + PRC(J,K)
   30 CONTINUE
C
      WRITE(6,2003) X, DX, NSTEP, KK
      WRITE(9,2003) X, DX, NSTEP, KK
      WRITE(6,2001)
```

```
      WRITE(6,2002) (AA(J),J=1,8)
      WRITE(9,2002) (AA(J),J=1,8)
      WRITE(6,2001)
      WRITE(6,2002) (PR(J),J=1,8)
      WRITE(9,2002) (PR(J),J=1,8)
      WRITE(6,2002)
C
      DO 200 K = 1, 34
      KMOD2 = 2*(K/2)
C
                                KFB = (K+1)/2
C     IF(KMOD2 .EQ. K)          KFB = K/2
C     REDUNDANT.
C
      WRITE(6,2007) K, KFB, RRC(K), RR(K), (PRC(J,K),J=1,8)
      WRITE(9,2007) K, KFB, RRC(K), RR(K), (PRC(J,K),J=1,8)
      IF(KMOD2 .EQ. K) WRITE(6,2004)
  200 CONTINUE
C
      WRITE(6,2000)
C
 1000 CONTINUE
C
C
 1999 FORMAT(1H1)
 2000 FORMAT(1H )
 1501 FORMAT(1H ,1PE10.3,11E11.3)
 2001 FORMAT(1H )
 2002 FORMAT(1H ,31X,1P8E12.4)
 2003 FORMAT(1H ,31X,1P2E12.4,50X,I7,3X,I3)
 2004 FORMAT(1H )
 2007 FORMAT(1H ,I2,1X,I2,1P2E12.4, 2X , 8E12.4)
      STOP
      END
@@GO.FT08F001 DD DSN=UF.B0035006.S1.KIN.EV1000.AB2C,
@@ DISP=(OLD,KEEP),DCB=(BLKSIZE=6072,LRECL=132,RECFM=FB)
@@GO.FT09F001 DD DUMMY
@@*GO.FT09F001 DD DSN=UF.B0035006.S1.KIN.EV1000.BB2C,
@@* DISP=(NEW,CATLG),DCB=(BLKSIZE=6072,LRECL=132,RECFM=FB),
@@* UNIT=SYSDA,SPACE=(6072,(100,20),RLSE)
@@GO.SYSIN  DD *
96
@*EOJ
-------------------------------
              PLOTLOW
-------------------------------
@@PLOTPROD JOB (7000,3791,20,40,0),DOCTORPAUL,REGION=700K,CLASS=2
@*PASSWORD
@*ROUTE  PRINT N1R0
@@ EXEC FORTXCG,LPARM='SIZE=600K',PLOT=
```

```
C
      REAL PLTTC(100,21)
      INTEGER*4 OPT
      REAL XVAL(100),YVAL(100),TEMP(2100)
C
C
C MAXIMUM NUMBER OF GRAPHS TO A PLOT EQUALS 20: DIMENSION OF KN
C
      DIMENSION KN(20), KNSIM(20), MSPECI(20)
      DIMENSION X(100), PRC(100,8,57)
C
      COMMON /PRC/ NPTSIN, X, PRC
      COMMON /TCPLT/ XVAL,YVAL,PLTTC
C
      NPTS = NPTSIN
C
C READ IN WIDTH AND HEIGHT OF PLOTS IN INCHES
      READ(5,45) WIDTH,HEIGHT
   45 FORMAT(2F5.2)
      WM1=WIDTH-1.
      HM1=HEIGHT-1.
C
C LOOP OVER NUMBER OF PLOTS,CONTROLED BY "END="
C
  100 CONTINUE
C     READ(5,40,END=9999) NT,OPT,RYMIN,RYMAX,NZEROT,TIMIN,TIMAX
C----     READ(5,40)          NT,OPT,RYMIN,RYMAX,NZEROT,TIMIN,TIMAX
C---- 40  FORMAT(2I3,2G14.7,I2,2G14.7)
      READ(5,*)           NT,OPT,RYMIN,RYMAX,NZEROT,TIMIN,TIMAX
C
      RPLTDX = (RYMAX - RYMIN)/HM1
C
      WRITE(6,29) NT
   29 FORMAT(' ',' NUMBER OF PRODUCTION RATE GRAPHS TO BE PLOTTED IS ',
     #I3,/)
      IF (OPT.EQ.0) WRITE(6,31)
      IF (OPT.EQ.1) WRITE(6,32) RYMIN,RPLTDX
      IF (OPT.EQ.1) WRITE(6,10032) RYMAX
10032 FORMAT(' ',' YMAX EQUALS ',G10.3)
      IF (NZEROT.EQ.1) WRITE(6,30)
   30 FORMAT(' ',' NO ZERO TIME IN DATA AND ALL TIMES ARE ',
     #' TO BE USED')
   31 FORMAT(' ',' PLOT SELF SCALED')
   32 FORMAT(' ',' PLOT SCALE SET WITH YMIN EQUAL TO ',
     #G10.2,' AND INCREMENT PER INCH SET TO ',G10.3)
C
      CALL PLOTS(WIDTH,HEIGHT,0,1,.5,.75)
      CALL LINEWT(-1)
      NCNT=NT+1
      READ(5,*)(KN(I),I=2,NCNT)
```

```
C
      READ(5,*) NPR
      READ(5,*) (MSPECI(I),I=1,NPR)
      READ(5,*) (KNSIM(I),I=1,NPR)
C
C
C-----------------------------------------------------------------------
C  READ IN THE DATA.  ASSIGN PLTTC VECTOR.  PLTTC(I,J) = T(I),J=1;
C  = C(I,J-1) FOR J = 2,NCNT WHERE NCNT = NT+1. NT=NO. OF SPECIES.
C  NPTS = NO. OF TIME POINTS.
C
      CALL KINRR
      NPTS = NPTSIN
      WRITE(6,*) NPTS
C
      DO 444 I = 1, NPTS
      PLTTC(I,1) = X(I)
      DO 444 J = 1, NPR
      PLTTC(I,J+1) = PRC(I,MSPECI(J),KNSIM(J))
  444 CONTINUE
C
C
C-----------------------------------------------------------------------
C INCREMENT KN IN ORDER TO MATCH INDICES OF PLTTC
C NOTE: PLTTC(I,J) J=1 -> TIME AND J=2,NCNT -> CONC. 1 -> NT
C
      KN(1)=1
      DO 1 I=2,NCNT
    1 KN(I)=KN(I)+1
C
C
      DO 2 JK=1,NCNT
        J=KN(JK)
        WRITE(6,8)
        WRITE(6,3) (PLTTC(I,J),I=1,NPTS)
    2 CONTINUE
    3 FORMAT(' ',10(1X,G10.3))
    8 FORMAT(' ',@@)
C
C   NZEROT IS SET EQUAL TO ONE IF THERE ARE NO ZERO TIMES
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  DAN FORGOT:
      NPT = NPTS
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
      IF(NZEROT.EQ.1) GO TO 6
C   ELIMINATE ZERO TIME FROM VECTOR PLTTC(I,1) ALONG WITH
C   CORRESPONDING PRODUCTION RATE PLTTC(I,J:J=2,NCNT)
C   ALSO USED TO ELIMINATE ALL TIMES LESS THAN TIMIN
C   AND ALL TIMES GREATER THAN TIMAX
      NPTM=0
```

:

```
      DO 7 I=1,NPTS
        IF (PLTTC(I,1).GT.TIMAX) GO TO 7
        NPTM=NPTM+1
    7 CONTINUE
      II=0
      NPT = NPTM
C   CORRECTION PFS
      DO 5 I=1,NPTM
        IF (PLTTC(I,1).GE.TIMIN) GO TO 5
          NPT=NPT-1
C   CORRECTION PFS
          II=II+1
      WRITE(6,333) I,NPTM,NPT,II,PLTTC(I,1),TIMIN,TIMAX
  333 FORMAT(' ',4I3,5G14.7)
    5 CONTINUE
      DO 4 JK=2,NCNT
      DO 4 K=1,NPT
        J=KN(JK)
        PLTTC(K,J)=PLTTC(K+II,J)
C   ****************************************
        IF (JK.EQ.2) PLTTC(K,1)=PLTTC(K+II,1)
    4 CONTINUE
    6 CONTINUE
C
C
C SCALE TIME(X) AXIS
C
      CALL POS(NPT,1)
      IF(OPT.EQ.1) GO TO 7777
      CALL LGSCAL(XVAL,WM1,1)
              PLTTC(NPT+1,1)=XVAL(NPT+1)
              PLTTC(NPT+2,1)=XVAL(NPT+2)
      WRITE(6,33) PLTTC(NPT+1,1),PLTTC(NPT+2,1)
   33 FORMAT(' ',' MINUMUM TIME EQUAL TO ',G14.7,
     #' WITH ',G14.7, 'DECADES PER INCH')
      GO TO 7778
C
C  OPTIONAL SCALE OVERRIDE
C
 7777 CONTINUE
      XVAL(NPT+1) = TIMIN
      PLTTC(NPT+1,1) = TIMIN
      XPLTDX = ALOG10(TIMAX/TIMIN) / WM1
      XVAL(NPT+2) = XPLTDX
      PLTTC(NPT+2,1) = XPLTDX
 7778 CONTINUE
C
C
C SCALE PRODUCTION RATE(Y) AXIS
C
```

```
      IF (OPT.EQ.1) GO TO 8002
C
      NTPT=1
      DO 8001 JK=2,NCNT
      J=KN(JK)
      DO 8001 I=1,NPT
C
C-----------------------------------------------------------------------
C
C     IF (PLTTC(I,J).LE.RYMIN) GO TO 8001
C
C  ESSENTIALLY TRIVIALIZE THIS PROCEDURE AS WELL, BUT USE IT FOR
C  MY OWN SIMPLER PURPOSES, IN THE MANNER OF BUCHLER:
C
      IF (PLTTC(I,J).LE.RYMIN) PLTTC(I,J) = RYMIN
      IF (PLTTC(I,J).GE.RYMAX) PLTTC(I,J) = RYMAX
C
C-----------------------------------------------------------------------
C
      TEMP(NTPT)=PLTTC(I,J)
      NTPT=NTPT+1
8001  CONTINUE
      NTPT=NTPT-1
      CALL SCALE(TEMP,HM1,NTPT,1)
            YMIN=TEMP(NTPT+1)
           PLTDX=TEMP(NTPT+2)
      WRITE(6,*) YMIN,PLTDX, RYMIN,RPLTDX
C
 8002 CONTINUE
C OPTIONAL SCALE OVERRIDE
C
      IF (OPT.EQ.1) YMIN=RYMIN
      IF (OPT.EQ.1) PLTDX=RPLTDX
C
C OUTLINE PLOT AND LABEL AXIS
C
      CALL AXIS(0.,0.,'PRODUCTION RATE (MOLE/CC/SEC)',29,HM1,90.,
     #YMIN,PLTDX)
      CALL LGAXIS(0.,0.,'      TIME (SEC)     ',-19,WM1,0.,PLTTC(NPT+1,1),
     #PLTTC(NPT+2,1))
      CALL PLOT(WM1,0.,3)
      CALL PLOT(WM1,HM1,2)
      CALL PLOT(0.,HM1,2)
C
C
C
      DO 222 JK=1,NCNT
        J=KN(JK)
        WRITE(6,8)
        WRITE(6,3) (PLTTC(I,J),I=1,NPT)
```

```
222   CONTINUE
C
      WRITE(6,*) NPT
      DO 8005 KJ=2,NCNT
        KJM=KJ-1
        J=KN(KJ)
        CALL POS(NPT,J)
      WRITE(6,*) NPT
        CALL PLOT(XVAL(1),YVAL(1),3)
C-----------------------------------------
C                    KSYM=MOD(J,13)
C                    LABEL=1
      LABEL=0
C-----------------------------------------
                   XVAL(NPT+1)=PLTTC(NPT+1,1)
                   XVAL(NPT+2)=PLTTC(NPT+2,1)
                   YVAL(NPT+1)=YMIN
                   YVAL(NPT+2)=PLTDX
C SPECIAL WRITE SECTION FOR DIAGNOSTICS
C
      JM1 = J - 1
      WRITE(6,8030) JM1
 8030 FORMAT(' ',' PLOT THE FOLLOWING PTS. FOR PROD. RATE NUM. ',I2)
      NPTP=NPT+2
      DO 8003 M=1,NPTP
        WRITE(6,8031) XVAL(M),YVAL(M)
 8003 CONTINUE
 8031 FORMAT(' ',2G14.7)
C
        IF (NPT.GT.1)CALL LGLINE(XVAL,YVAL,NPT,1,LABEL,
     #  KSYM,1)
 8005 CONTINUE
      CALL PLOT(0.,0.,999)
C     ........................................      GOTO 100
9999  STOP
      END
      SUBROUTINE POS(NPT,K)
      REAL PLTTC(100,21)
      REAL XVAL(100),YVAL(100)
      COMMON /TCPLT/ XVAL,YVAL,PLTTC
C    SUBROUTINE LOADS PLOT VECTORS FOR PLOT & SCALES THEM
      DO 2 I=1,NPT
        YVAL(I)=PLTTC(I,K)
        XVAL(I)=PLTTC(I,1)
    2 CONTINUE
C
      RETURN
      END
@*INCLUDE PL.KINRR   20035006.12
@@*
```

```
@@*GO.SYSVECTR DD SPACE=(TRK,(200,100),RLSE)
@@*
@@GO.SYSIN DD *
10.0 13.0
@@*  17   1        -6.0E-10     3.0E-10    0       1.0E-05    1.0E+02
@@*1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17
@@* 17
@@*1,2,3,4,5,6,7,8,1,2,3,4,5,6,7,8,1
@@*55,55,55,55,55,55,55,55,56,56,56,56,56,56,56,56,57
@@*  08   1        -12.E-10     12.E-10    0       1.0E-05    1.0E+02
@@*1,2,3,4,5,6,7,8
@@* 08
@@*1,2,3,4,5,6,7,8
@@*53,53,53,53,53,53,53,53,53
@@*
@@* 05  1        -6.0E-10     3.0E-10    0       1.0E-05        1.0E+02
@@*1,2,3,4,5
@@* 05
@@*2,2,2,2,2
@@*36,38,44,48,51
@@*
@@* 07  1        -2.5E-10     3.5E-10    0       1.0E-05        1.0E+02
@@*1,2,3,4,5,6,7
@@* 07
@@*8,8,8,8,8,8,8
@@*35,41,42,44,45,46,50
@@*
@@* 06  1        -3.5E-10     2.5E-10    0       1.0E-05        1.0E+02
@@*1,2,3,4,5,6
@@* 06
@@*6,6,6,6,6,6
@@*35,36,37,42,49,50
@@*
@@* 10  1        -6.0E-10     6.0E-10    0       1.0E-05        1.0E+02
@@*1,2,3,4,5,6,7,8,9,10
@@* 10
@@*1,1,1,1,1,1,1,1,1,1
@@*35,36,38,40,41,43,44,48,49,51
@@*
@@* 11  1        -6.0E-10     6.0E-10    0       1.0E-05        1.0E+02
@@*1,2,3,4,5,6,7,8,9,10,11
@@* 11
@@*7,7,7,7,7,7,7,7,7,7,7
@@*35,36,37,38,39,40,42,43,45,47,49
@@*
@@* 08  1        -3.0E-10     3.0E-10    0       1.0E-05        1.0E+02
@@*1,2,3,4,5,6,7,8
@@* 08
@@*4,4,4,4,4,4,4,4
@@*39,41,42,43,44,45,46,48
```

```
@@*
@@*  04   1        -1.6E-12      2.0E-12    0        1.0E-05        1.0E+02
@@*1,2,3,4
@@*  04
@@*5,5,5,5
@@*39,46,47,48
@@*
@@*  05   1        -3.0E-10      9.0E-10    0        1.0E-05        1.0E+02
@@*1,2,3,4,5
@@*  05
@@*3,3,3,3,3
@@*37,38,39,40,45
@@*
@@GO.FT08F001 DD DSN=UF.B0035006.S1.KIN.EV1000.AB9C.DISP=OLD
@@*  DCB=(RECFM=FB,BLKSIZE=6072,LRECL=132)
@@*NEED NOT MENTION, RECORDED IN CATALOG, BUT IF YOU DO, COMMA
@@*MUST GO IN PRECEDING LINE
@@GO.FT09F001 DD *
96
@@GO.FT15F001 DD SYSOUT=A
@@*  WHAT IS THIS FOR?
@@*
@@*
@@*  EXEC PLOT,SIZE=500
@@   EXEC PLOT
@@*
@*EOJ
-------------------------------
                DATAATM
-------------------------------
@@GO.SYSIN DD *
10.0 13.0
@@*  16   1        -2.0E-04      2.8E-04    0        1.0E-09    1.0E-02
@@*1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16
@@*  16
@@*1,2,3,4,5,7,8,1,2,3,4,5,6,7,8,1
@@*55,55,55,55,55,55,55,55,56,56,56,56,56,56,56,56,57
@@*
@@*  17   1        -9.0E-04      3.0E-04    0        1.0E-09    1.0E-02
@@*1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17
@@*  17
@@*1,2,3,4,5,6,7,8,1,2,3,4,5,6,7,8,1
@@*55,55,55,55,55,55,55,55,56,56,56,56,56,56,56,56,57
@@*
@@*  08   1        -12.E-04      12.E-04    0        1.0E-09    1.0E-02
@@*1,2,3,4,5,6,7,8
@@*  08
@@*1,2,3,4,5,6,7,8
@@*53,53,53,53,53,53,53,53
@@*
```

```
@@* 05  1          -1.2E-04      1.2E-04    0          1.0E-09        1.0E-02
@@*1,2,3,4,5
@@* 05
@@*2,2,2,2,2
@@*36,38,44,48,51
@@*
@@* 07  1          -3.0E-04      1.8E-04    0          1.0E-09        1.0E-02
@@*1,2,3,4,5,6,7
@@* 07
@@*8,8,8,8,8,8,8
@@*35,41,42,44,45,46,50
@@*
@@* 06  1          -9.0E-05      3.0E-05    0          1.0E-09        1.0E-02
@@*1,2,3,4,5,6
@@* 06
@@*6,6,6,6,6,6
@@*35,36,37,42,49,50
@@*
@@* 10  1          -9.0E-04      3.0E-04    0          1.0E-09        1.0E-02
@@*1,2,3,4,5,6,7,8,9,10
@@* 10
@@*1,1,1,1,1,1,1,1,1,1
@@*35,36,38,40,41,43,44,48,49,51
@@*
@@* 11  1          -12.E-04      6.0E-04    0          1.0E-09        1.0E-02
@@*1,2,3,4,5,6,7,8,9,10,11
@@* 11
@@*7,7,7,7,7,7,7,7,7,7,7
@@*35,36,37,38,39,40,42,43,45,47,49
@@*
@@* 08  1          -3.0E-04      3.0E-04    0          1.0E-09        1.0E-02
@@*1,2,3,4,5,6,7,8
@@* 08
@@*4,4,4,4,4,4,4,4
@@*39,41,42,43,44,45,46,48
@@*
@@* 04  1          -3.0E-04      3.0E-04    0          1.0E-09        1.0E-02
@@*1,2,3,4
@@* 04
@@*5,5,5,5
@@*39,46,47,48
@@*
@@* 05  1          -3.0E-04      9.0E-04    0          1.0E-09        1.0E-02
@@*1,2,3,4,5
@@* 05
@@*3,3,3,3,3
@@*37,38,39,40,45
@@*
@@GO.FT08F001 DD DSN=UF.B0035006.S1.KIN.EV1000.AB30.DISP=OLD
@@* DCB=(RECFM=FB,BLKSIZE=6072,LRECL=132)
```

```
@@*NEED NOT MENTION, RECORDED IN CATALOG, BUT IF YOU DO, COMMA
@@*MUST GO IN PRECEDING LINE
@@GO.FT09F001 DD *
96
@@GO.FT15F001 DD SYSOUT=A
@@* WHAT IS THIS FOR?
@@*
@@*
@@* EXEC PLOT,SIZE=500
@@  EXEC PLOT
@@*
@*EOJ
-------------------------------
              DATALIQ
-------------------------------
@@GO.SYSIN DD *
10.0 13.0
@@*  15   1        -0.8E-11    1.6E-11    0       1.0E-07    1.0E+00
@@*1,2,3,4,5,6,7,8,9,10,11,12,13,14,15
@@* 15
@@*1,2,3,4,5,7,8,1,2,3,4,6,7,8,1
@@*55,55,55,55,55,55,55,56,56,56,56,56,56,56,57
@@*  17  1       -3.0E-10     0.6E-10   0       1.0E-07    1.0E+00
@@*1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17
@@* 17
@@*1,2,3,4,5,6,7,8,1,2,3,4,5,6,7,8,1
@@*55,55,55,55,55,55,55,55,56,56,56,56,56,56,57
@@*  08  1       -3.0E-10     3.0E-10   0       1.0E-07    1.0E+00
@@*1,2,3,4,5,6,7,8
@@* 08
@@*1,2,3,4,5,6,7,8
@@*53,53,53,53,53,53,53,53,53
@@*
@@* 05  1        -1.2E-12     9.6E-12   0       1.0E-07        1.0E+00
@@*1,2,3,4,5
@@* 05
@@*2,2,2,2,2
@@*36,38,44,48,51
@@*
@@* 07  1        -8.4E-12     2.4E-12   0       1.0E-07        1.0E+00
@@*1,2,3,4,5,6,7
@@* 07
@@*8,8,8,8,8,8,8
@@*35,41,42,44,45,46,50
@@*
@@* 06  1        -1.5E-11     1.5E-11   0       1.0E-07        1.0E+00
@@*1,2,3,4,5,6
@@* 06
@@*6,6,6,6,6,6
@@*35,36,37,42,49,50
```

```
@@*
@@* 10  1          -3.0E-10      0.6E-10    0         1.0E-07         1.0E+00
@@*1,2,3,4,5,6,7,8,9,10
@@* 10
@@*1,1,1,1,1,1,1,1,1,1
@@*35,36,38,40,41,43,44,48,49,51
@@*
@@* 11  1          -3.0E-10      0.6E-10    0         1.0E-07         1.0E+00
@@*1,2,3,4,5,6,7,8,9,10,11
@@* 11
@@*7,7,7,7,7,7,7,7,7,7 ,7
@@*35,36,37,38,39,40,42,43,45,47,49
@@*
@@* 08  1          -4.0E-12      8.0E-12    0         1.0E-07         1.0E+00
@@*1,2,3,4,5,6,7,8
@@* 08
@@*4,4,4,4,4,4,4,4
@@*39,41,42,43,44,45,46,48
@@*
@@* 04  1          -0.2E-11      4.6E-11    0         1.0E-07         1.0E+00
@@*1,2,3,4
@@* 04
@@*5,5,5,5
@@*39,46,47,48
@@*
@@* 05  1          -3.0E-10      3.0E-10    0         1.0E-07         1.0E+00
@@*1,2,3,4,5
@@* 05
@@*3,3,3,3,3
@@*37,38,39,40,45
@@*
@@GO.FT08F001 DD DSN=JF.B0035006.S1.KIN.EV1000.AB21,DISP=OLD
@@* DCB=(RECFM=FB,BLKSIZE=6072,LRECL=132)
@@*NEED NOT MENTION, RECORDED IN CATALOG, BUT IF YOU DO, COMMA
@@*MUST GO IN PRECEDING LINE
@@GO.FT09F001 DD *
96
@@GO.FT15F001 DD SYSOUT=A
@@* WHAT IS THIS FOR?
@@*
@@*
@@* EXEC PLOT,SIZE=500
@@  EXEC PLOT
@@*
@*EOJ
-----------------------------
 PL.KINRR (USED BY LOW & LIQ)
-----------------------------
      SUBROUTINE KINRR
C-----------------------------------------------------------------------------
```

```
C   1. CHECK MASS BALANCE IN KINETIC PROGRAM
C   2. DISPLAY REACTION RATES AND PRODUCTION RATES
C
C-----------------------------------------------------------------------------
C
      DIMENSION A(11,1), AH(1), AO(1), YI(12,1), RX(1)
      DIMENSION YH(1), YO(1), YTH(1), YTO(1)
C
      DIMENSION RRC(34), RR(34), PRC(100,8,57), ISTOI(8,34)
      DIMENSION          RRFB(17)
      DIMENSION                   X(100)
      DIMENSION IST(8,17), PR(100,8), PRTOT(100,8)
      DIMENSION PRTOAB(100,8)
      DIMENSION AA(11)
C
      COMMON /PRC/ IPAGE, X, PRC
C
      EQUIVALENCE (A(1),AA(1))
      EQUIVALENCE (PR(1), PRC(1,1,52))
      EQUIVALENCE (PRTOT(1), PRC(1,1,53))
      EQUIVALENCE (PRTOAB(1), PRC(1,1,54))
C
C   J = 1  H       POS. YIELD
C       2  H2      POS. YIELD
C       3  H2O     NEG. YIELD
C       4  HO2
C       5  H2O2
C       6  O       POS. YIELD
C       7  OH      POS. YIELD
C       8  O2
C
      CALL ERRSET(208,2000,-1,1)
C
C
C
C   HARDWIRED.  TEMPORARY.  400 K:
      DATA RRC/  1.244E05, 6.294E12, 9.954E07, 5.300E08,
     1 3.187E03, 7.910E11, 7.729E02, 3.359E10, 1.038E12, 3.432E-5,
     2 9.26E-42, 8.812E17, 5.837E15, 1.90E-10, 1.424E13, 7.54E-18,
     3 2.299E13, 1.472E-9, 1.041E13, 1.43E-18, 1.424E13, 2.76E-26,
     4 2.00E-10, 2.843E12, 1.65E-08, 5.380E17, 1.514E10, 43.84,
     5 1.000E16, 4.19E-40, 7.45E-48, 8.743E14, 7.66E-39, 3.02E15 /
C
C   HARDWIRED.  TEMPORARY.  300 K:  (REMEMBER TO COME IN HERE AND DO
C   MINOR SURGERY WHEN YOU WANT IT CHANGED TO THIS TEMPERATURE.  IF AND
C   WHEN YOU WANT ANY TEMPERATURE, MODIFY THIS.
C
C     DATA RRC/ 1.09E2, 4.73E12, 1.76E6, 2.16E7, 1.45, 5.00E11,
C    1 1.55E-1, 3.87E9, 4.88E11, 3.64E-11, 7.00E-60, 1.57E18,
C    2 8.88E15, 8.30E-19, 9.36E12, 3.68E-28, 1.04E13, 7.32E-17,
```

:

```
C     3 7.76E12, 4.26E-29, 9.36E12, 9.74E-40, 3.42E-18, 1.87E12,
C     4 8.52E-17, 4.51E18, 3.15E9, 1.72E-2, 1.00E16, 0., 0.,
C     5 9.47E14, 2.50E-56, 3.02E15 /
C
      DATA IST/ -1, 0, 0, 0, 0, 1, 1,-1,
     2           1,-1, 0, 0, 0,-1, 1, 0,
     3           0, 0,-1, 0, 0,-1, 2, 0,
     4          -1, 1,-1, 0, 0, 0, 1, 0,
     5           0, 0, 1,-1, 1, 0,-1, 0,
     6           1, 0,-1, 0, 0, 0, 1, 0,
     7          -1, 0, 0, 0, 1, 0, 0,-1,
     8           0, 0, 0, 0,-1,-1, 1, 1,
     9          -1, 0, 0, 0,-1, 0, 2, 0,
     X          -1, 1, 0, 0,-1, 0, 0, 1,
     1           0, 0, 1, 0,-1, 0,-1, 1,
     2           0, 0, 0,-1, 2, 0, 0,-1,
     3           0, 0, 0,-1, 0, 0, 2, 0,
     4          -1, 1, 0,-1, 1, 0, 0, 0,
     5          -1, 0, 0, 0, 0,-1, 1, 0,
     6           0, 0, 0, 0, 0, 2, 0,-1,
     7           2,-1, 0, 0, 0, 0, 0, 0/
C
C  CORRECT SWITCH OF H2O2 WITH HO2 (INADVERTENT)
      DO 1025 I = 1,17
      ISTSAV = IST(4,I)
      IST(4,I) = IST(5,I)
 1025 IST(5,I) = ISTSAV
C
      DO 25 K = 1,17
      DO 25 J = 1,8
      KE = 2*K
      KO = KE-1
      ISTOI(J,KO) = IST(J,K)
      ISTOI(J,KE) = -IST(J,K)
   25 CONTINUE
C
      NS = 8
C
C     AH2O = 0.99626E-08
C     XAH2O = 0.00001E-08
C
C-------------READ STARTING SECTION-----------------------------------------
C
      NSKIPM = 11
      DO 210 I = 1,NSKIPM
      READ(8,1) QAQ
  210 CONTINUE
    1 FORMAT(A4)
C
C  NOW READ YI(J,1)  (THE YIELDS)
```

```
      READ(8,3) RX(1),(YI(J,1),J=1,8)
    3 FORMAT(T7,1P9E11.4)
C
      NSKIPM = 8
      DO 310 I = 1,NSKIPM
      READ(8,1) QAQ
  310 CONTINUE
C
C-----------------------------------------------------------------------
C  HERE START READ LOOP
C
      READ(9,*) IPAGE
      DO 1000 KK = 1,IPAGE
C
      NLOOP = 6
      DO 410 I = 1,NLOOP
      READ(8,1) QAQ
  410 CONTINUE
C  NOW READ X  (TIME)
      XSAV = X(KK)
      READ(8,4) X(KK)
    4 FORMAT(T5,E14.7)
C  NOW READ DX (IN CASE)
      DXSAV = DX
      READ(8,5) DX, NSTEP
    5 FORMAT(T7,E14.7,16X,I7)
C*****************************************      READ(8,1) QAQ
C  NOW READ A(J,1) (THE CONCENTRATIONS)
      READ(8,6) (A(J,1),J=1,8)
    6 FORMAT(T13,1P8E11.4)
C
      IF (KK .NE. 1) GO TO 252
      AH2O = A(3,1)
      XAH2O = .0001*AH2O
  252 CONTINUE
C
C END OF READ ---------------------------------------------------------
C
      MPSI = 1
      DO 100 I = 1, MPSI
C
      YH(I) = YI(1,I) + 2.*YI(2,I) + YI(7,I)
      YTH(I) = YH(I) + 2.*YI(3,I)
C
      YO(I) = YI(6,I) + YI(7,I)
      YTO(I) = YO(I) + YI(3,I)
C
      YI(9,I) = YH(I)
      YI(10,I) = YTH(I)
      YI(11,I) = YO(I)
```

```
      YI(12,I) = YTO(I)
C
      A(11,I) = A(3,I) - AH2O
C*********************      IF(A(11,I) .LT. XAH2O) A(13,I) = 0.
C  BELOW THE LIMIT OF NUMERICAL ROUNDOFF ERROR
C
      AH(I) = A(1,I) + 2.*A(2,I) + 2.*A(11,I) + A(4,I) + 2.*A(5,I) +
     @  A(7,I)
      AO(I) = A(11,I) + 2.*A(4,I) + 2.*A(5,I) + A(6,I) + A(7,I) +
     $  2.*A(8,I)
C
      A(9,I) = AH(I)
      A(10,I) = AO(I)
C
C     WRITE(6,1999)
C     WRITE(6,1501) (YI(J,I),J=1,12)
C     WRITE(9,1501) (YI(J,I),J=1,12)
C     WRITE(6,2002)
C     WRITE(6,1501) (A(J,I),J=1,11)
C     WRITE(9,1501) (A(J,I),J=1,11)
C     WRITE(6,2002)
C
      RAT = 0.
      IF(AO(I) .EQ. 0.) GO TO 272
      RAT = AH(I)/AO(I)
      CORAT = RAT - 2.
  272 CONTINUE
C
C     WRITE(6,1501) AH(I), AO(I), RAT, CORAT
C     WRITE(9,1501) AH(I), AO(I), RAT, CORAT
C     WRITE(6,2000)
  100 CONTINUE
C
C
C   CORRECT SWITCH OF H2O2 AND HO2 (INADVERTENT)
      AASAV = AA(4)
      AA(4) = AA(5)
      AA(5) = AASAV
C
      RR(1) = RRC(1)*AA(1)*AA(8)
      RR(2) = RRC(2)*AA(6)*AA(7)
      RR(3) = RRC(3)*AA(2)*AA(6)
      RR(4) = RRC(4)*AA(1)*AA(7)
      RR(5) = RRC(5)*AA(3)*AA(6)
      RR(6) = RRC(6)*AA(7)*AA(7)
      RR(7) = RRC(7)*AA(3)*AA(1)
      RR(8) = RRC(8)*AA(2)*AA(7)
      RR(9) = RRC(9)*AA(4)*AA(7)
      RR(10) = RRC(10)*AA(3)*AA(5)
      RR(11) = RRC(11)*AA(3)*AA(3)
```

```
      RR(12) = RRC(12)*AA(1)*AA(7)*AA(3)
      RR(13) = RRC(13)*AA(1)*AA(8)*AA(3)
      RR(14) = RRC(14)*AA(5)*AA(3)
      RR(15) = RRC(15)*AA(5)*AA(6)
      RR(16) = RRC(16)*AA(7)*AA(8)
      RR(17) = RRC(17)*AA(5)*AA(1)
      RR(18) = RRC(18)*AA(7)*AA(7)
      RR(19) = RRC(19)*AA(5)*AA(1)
      RR(20) = RRC(20)*AA(2)*AA(8)
      RR(21) = RRC(21)*AA(5)*AA(7)
      RR(22) = RRC(22)*AA(3)*AA(8)
      RR(23) = RRC(23)*AA(4)*AA(8)
      RR(24) = RRC(24)*AA(5)*AA(5)
      RR(25) = RRC(25)*AA(4)*AA(3)
      RR(26) = RRC(26)*AA(7)*AA(7)*AA(3)
      RR(27) = RRC(27)*AA(4)*AA(1)
      RR(28) = RRC(28)*AA(5)*AA(2)
      RR(29) = RRC(29)*AA(6)*AA(1)*AA(3)
      RR(30) = RRC(30)*AA(7)*AA(3)
      RR(31) = RRC(31)*AA(8)*AA(3)
      RR(32) = RRC(32)*AA(6)*AA(6)*AA(3)
      RR(33) = RRC(33)*AA(2)*AA(3)
      RR(34) = RRC(34)*AA(1)*AA(1)*AA(3)
C
C  SWITCH BACK
      AASAV = AA(4)
      AA(4) = AA(5)
      AA(5) = AASAV
C
C
C
      DO 30 J = 1, 8
      PR(KK,J) = 0.
      DO 29 K = 1, 34
      PRC(KK,J,K) = RR(K)*ISTOI(J,K)
      PR(KK,J) = PR(KK,J) + PRC(KK,J,K)
   29 CONTINUE
      PRTOT(KK,J) = PR(KK,J) + YI(J,1)
      PRTOAB(KK,J) = ABS(PRTOT(KK,J))
   30 CONTINUE
C
C++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C  TWO-WAY REACTION  PRODUCTION RATES: ----------------------
C
      DO 40 J = 1, 8
      DO 40 KILROY = 1, 17
      KE = KILROY * 2
      KO = KE - 1
      PRC(KK,J,KILROY+34) = PRC(KK,J,KO) + PRC(KK,J,KE)
   40 CONTINUE
```

```
C++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C  TWO-WAY REACTION RATES
C
      DO 1010 IFB = 1,17
 1010 RRFB(IFB) = RR(2*IFB-1) - RR(2*IFB)
C
      DO 1020 IFB = 1,17
      IFBMD8 =  IFB/8
      KNSIM = 55 + IFBMD8
      IFBRMD = IFB - (IFB/8)*8
 1020 PRC(KK,IFBRMD,55+IFBMD8) = RRFB(IFB)
C
C  WHEN YOU GOT LEMONS, MAKE LEMONADE:  I WANT TO SEND 17 QUANTITIES
C  INDEPENDENT OF SPECIES THROUGH PRC(100,8,X).  RATHER THAN JUST USE THE
C  FIRST SLOT OUT OF 8 FOR 17 EXTRA IN X, DIVIDE 17 INTO GROUPS OF 8 PLUS
C  A REMAINDER.
C
C++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C
C     WRITE(6,2003) X(KK), DX, NSTEP, KK
C     WRITE(9,2003) X(KK), DX, NSTEP, KK
C     WRITE(6,2001)
C     WRITE(6,2002) (AA(J),J=1,8)
C     WRITE(9,2002) (AA(J),J=1,8)
C     WRITE(6,2001)
C     WRITE(6,2002) (PR(KK,J),J=1,8)
C     WRITE(9,2002) (PR(KK,J),J=1,8)
C     WRITE(6,2002)
C
CCCCCCCCCCCCCCCCC      DO 200 K = 1, 34
CCCCCCCCCCCCCCCCC      KMOD2 = 2*(K/2)
C
CCCCCCCCCCCCCCCCC                              KFB = (K+1)/2
CCCCCCCCCCCCCCCCC      IF(KMOD2 .EQ. K)        KFB = K/2
CCCCCCCCCCCCCCCCC      REDUNDANT.
C
CCCCCCCCCCCCCCCCC      WRITE(6,2007) K, KFB, RRC(K), RR(K), (PRC(KK,J,K),J=1,8)
CCCCCCCCCCCCCCCCC      WRITE(9,2007) K, KFB, RRC(K), RR(K), (PRC(KK,J,K),J=1,8)
CCCCCCCCCCCCCCCCC      IF(KMOD2 .EQ. K) WRITE(6,2004)
CCCCCCCCCCCCCCCCC 200 CONTINUE
C
CCCCCCCCCCCCCCCCC      WRITE(6,2000)
C
 1000 CONTINUE
C
C
 1999 FORMAT(1H1)
 2000 FORMAT(1H )
 1501 FORMAT(1H ,1PE10.3,11E11.3)
 2001 FORMAT(1H )
```

```
 2002 FORMAT(1H ,31X,1P8E12.4)
 2003 FORMAT(1H ,31X,1P2E12.4,50X,I7,3X,I3)
 2004 FORMAT(1H )
 2007 FORMAT(1H ,I2,1X,I2,1P2E12.4, 2X , 8E12.4)
      RETURN
      END
-----------------------------
    PL.KNRAT (USED BY ATM)
-----------------------------
      SUBROUTINE KINRR
C-----------------------------------------------------------------------------
C  1. CHECK MASS BALANCE IN KINETIC PROGRAM
C  2. DISPLAY REACTION RATES AND PRODUCTION RATES
C
C-----------------------------------------------------------------------------
C
      DIMENSION A(11,1), AH(1), AO(1), YI(12,1), RX(1)
      DIMENSION YH(1), YO(1), YTH(1), YTO(1)
C
      DIMENSION RRC(34), RR(34), PRC(100,8,57), ISTDI(8,34)
      DIMENSION          RRFB(17)
      DIMENSION                    X(100)
      DIMENSION IST(8,17), PR(100,8), PRTOT(100,8)
      DIMENSION PRTOAB(100,8)
      DIMENSION AA(11)
C
      COMMON /PRC/ IPAGE, X, PRC
C
      EQUIVALENCE (A(1),AA(1))
      EQUIVALENCE (PR(1), PRC(1,1,52))
      EQUIVALENCE (PRTOT(1), PRC(1,1,53))
      EQUIVALENCE (PRTOAB(1), PRC(1,1,54))
C
C  J = 1  H       POS. YIELD
C      2  H2      POS. YIELD
C      3  H2O     NEG. YIELD
C      4  HO2
C      5  H2O2
C      6  O       POS. YIELD
C      7  OH      POS. YIELD
C      8  O2
C
      CALL ERRSET(208,2000,-1,1)
C
C
C
C  HARDWIRED.  TEMPORARY.  400 K:
      DATA RRC/  1.244E05, 6.294E12, 9.954E07, 5.300E08,
     1 3.187E03, 7.910E11, 7.729E02, 3.359E10, 1.038E12, 3.432E-5,
     2 9.26E-42, 8.812E17, 5.837E15, 1.90E-10, 1.424E13, 7.54E-18,
```

```
     3 2.299E13, 1.472E-9, 1.041E13, 1.43E-18, 1.424E13, 2.76E-26,
     4 2.00E-10, 2.843E12, 1.65E-08, 5.380E17, 1.514E10, 43.84,
     5 1.000E16, 4.19E-40, 7.45E-48, 8.743E14, 7.66E-39, 3.02E15 /
C
C   HARDWIRED.  TEMPORARY.  300 K:  (REMEMBER TO COME IN HERE AND DO
C   MINOR SURGERY WHEN YOU WANT IT CHANGED TO THIS TEMPERATURE.  IF AND
C   WHEN YOU WANT ANY TEMPERATURE, MODIFY THIS.
C
C      DATA RRC/ 1.09E2, 4.73E12, 1.76E6, 2.16E7, 1.45, 5.00E11,
C     1 1.55E-1, 3.87E9, 4.88E11, 3.64E-11, 7.00E-60, 1.57E18,
C     2 8.88E15, 8.30E-19, 9.36E12, 3.68E-28, 1.04E13, 7.32E-17,
C     3 7.76E12, 4.26E-29, 9.36E12, 9.74E-40, 3.42E-18, 1.87E12,
C     4 8.52E-17, 4.51E18, 3.15E9, 1.72E-2, 1.00E16, 0., 0.,
C     5 9.47E14, 2.50E-56, 3.02E15 /
C
      DATA IST/ -1, 0, 0, 0, 0, 1, 1,-1,
     2           1,-1, 0, 0, 0,-1, 1, 0,
     3           0, 0,-1, 0, 0,-1, 2, 0,
     4          -1, 1,-1, 0, 0, 0, 1, 0,
     5           0, 0, 1,-1, 1, 0,-1, 0,
     6           1, 0,-1, 0, 0, 0, 1, 0,
     7          -1, 0, 0, 0, 1, 0, 0,-1,
     8           0, 0, 0, 0,-1,-1, 1, 1,
     9          -1, 0, 0, 0,-1, 0, 2, 0,
     X          -1, 1, 0, 0,-1, 0, 0, 1,
     1           0, 0, 1, 0,-1, 0,-1, 1,
     2           0, 0, 0,-1, 2, 0, 0,-1,
     3           0, 0, 0,-1, 0, 0, 2, 0,
     4          -1, 1, 0,-1, 1, 0, 0, 0,
     5          -1, 0, 0, 0, 0,-1, 1, 0,
     6           0, 0, 0, 0, 0, 2, 0,-1,
     7           2,-1, 0, 0, 0, 0, 0, 0/
C
C   CORRECT SWITCH OF H2O2 WITH HO2 (INADVERTENT)
      DO 1025 I = 1,17
      ISTSAV = IST(4,I)
      IST(4,I) = IST(5,I)
 1025 IST(5,I) = ISTSAV
C
      DO 25 K = 1,17
      DO 25 J = 1,8
      KE = 2*K
      KO = KE-1
      ISTOI(J,KO) = IST(J,K)
      ISTOI(J,KE) = -IST(J,K)
   25 CONTINUE
C
      NS = 8
C
C     AH2O = 0.99626E-08
```

```
C      XAH2O = 0.00001E-08
C
C-------------READ STARTING SECTION-----------------------------------------
C
      NSKIPM = 11
      DO 210 I = 1,NSKIPM
      READ(8,1) QAQ
  210 CONTINUE
    1 FORMAT(A4)
C
C  NOW READ YI(J,1)  (THE YIELDS)
      READ(8,3) RX(1),(YI(J,I),J=1,8)
    3 FORMAT(T7,1P9E11.4)
C
      NSKIPM = 8
      DO 310 I = 1,NSKIPM
      READ(8,1) QAQ
  310 CONTINUE
C
C-----------------------------------------------------------------------
C  HERE START READ LOOP
C
      READ(9,*) IPAGE
      DO 1000 KK = 1,IPAGE
C
      NLOOP = 6
      DO 410 I = 1,NLOOP
      READ(8,1) QAQ
  410 CONTINUE
C  NOW READ X  (TIME)
      XSAV = X(KK)
      READ(8,4) X(KK)
    4 FORMAT(T5,E14.7)
C  NOW READ DX (IN CASE)
      DXSAV = DX
      READ(8,5) DX, NSTEP
    5 FORMAT(T7,E14.7,16X,I7)
C*********************************************      READ(8,1) QAQ
C  NOW READ A(J,1) (THE CONCENTRATIONS)
      READ(8,6) (A(J,1),J=1,8)
    6 FORMAT(T16,1P8E11.4)
C
      IF (KK .NE. 1) GO TO 252
      AH2O = A(3,1)
      XAH2O = .0001*AH2O
  252 CONTINUE
C
C END OF READ ---------------------------------------------------------
C
      MPSI = 1
```

```
      DO 100 I = 1, MPSI
C
      YH(I) = YI(1,I) + 2.*YI(2,I) + YI(7,I)
      YTH(I) = YH(I) + 2.*YI(3,I)
C
      YO(I) = YI(6,I) + YI(7,I)
      YTO(I) = YO(I) + YI(3,I)
C
      YI(9,I) = YH(I)
      YI(10,I) = YTH(I)
      YI(11,I) = YO(I)
      YI(12,I) = YTO(I)
C
      A(11,I) = A(3,I) - AH2O
C.......................      IF(A(11,I) .LT. XAH2O) A(13,I) = 0.
C  BELOW THE LIMIT OF NUMERICAL ROUNDOFF ERROR
C
      AH(I) = A(1,I) + 2.*A(2,I) + 2.*A(11,I) + A(4,I) + 2.*A(5,I) +
     @  A(7,I)
      AO(I) = A(11,I) + 2.*A(4,I) + 2.*A(5,I) + A(6,I) + A(7,I) +
     $  2.*A(8,I)
C
      A(9,I) = AH(I)
      A(10,I) = AO(I)
C
C     WRITE(6,1999)
C     WRITE(6,1501) (YI(J,I),J=1,12)
C     WRITE(9,1501) (YI(J,I),J=1,12)
C     WRITE(6,2002)
C     WRITE(6,1501) (A(J,I),J=1,11)
C     WRITE(9,1501) (A(J,I),J=1,11)
C     WRITE(6,2002)
C
      RAT = 0.
      IF(AO(I) .EQ. 0.) GO TO 272
      RAT = AH(I)/AO(I)
      CORAT = RAT - 2.
  272 CONTINUE
C
C     WRITE(6,1501) AH(I), AO(I), RAT, CORAT
C     WRITE(9,1501) AH(I), AO(I), RAT, CORAT
C     WRITE(6,2000)
  100 CONTINUE
C
C
C  CORRECT SWITCH OF H2O2 AND HO2 (INADVERTENT)
      AASAV = AA(4)
      AA(4) = AA(5)
      AA(5) = AASAV
C
```

```
      RR(1) = RRC(1)*AA(1)*AA(8)
      RR(2) = RRC(2)*AA(6)*AA(7)
      RR(3) = RRC(3)*AA(2)*AA(6)
      RR(4) = RRC(4)*AA(1)*AA(7)
      RR(5) = RRC(5)*AA(3)*AA(6)
      RR(6) = RRC(6)*AA(7)*AA(7)
      RR(7) = RRC(7)*AA(3)*AA(1)
      RR(8) = RRC(8)*AA(2)*AA(7)
      RR(9) = RRC(9)*AA(4)*AA(7)
      RR(10) = RRC(10)*AA(3)*AA(5)
      RR(11) = RRC(11)*AA(3)*AA(3)
      RR(12) = RRC(12)*AA(1)*AA(7)*AA(3)
      RR(13) = RRC(13)*AA(1)*AA(8)*AA(3)
      RR(14) = RRC(14)*AA(5)*AA(3)
      RR(15) = RRC(15)*AA(5)*AA(6)
      RR(16) = RRC(16)*AA(7)*AA(8)
      RR(17) = RRC(17)*AA(5)*AA(1)
      RR(18) = RRC(18)*AA(7)*AA(7)
      RR(19) = RRC(19)*AA(5)*AA(1)
      RR(20) = RRC(20)*AA(2)*AA(8)
      RR(21) = RRC(21)*AA(5)*AA(7)
      RR(22) = RRC(22)*AA(3)*AA(8)
      RR(23) = RRC(23)*AA(4)*AA(8)
      RR(24) = RRC(24)*AA(5)*AA(5)
      RR(25) = RRC(25)*AA(4)*AA(3)
      RR(26) = RRC(26)*AA(7)*AA(7)*AA(3)
      RR(27) = RRC(27)*AA(4)*AA(1)
      RR(28) = RRC(28)*AA(5)*AA(2)
      RR(29) = RRC(29)*AA(6)*AA(1)*AA(3)
      RR(30) = RRC(30)*AA(7)*AA(3)
      RR(31) = RRC(31)*AA(8)*AA(3)
      RR(32) = RRC(32)*AA(6)*AA(6)*AA(3)
      RR(33) = RRC(33)*AA(2)*AA(3)
      RR(34) = RRC(34)*AA(1)*AA(1)*AA(3)
C
C   SWITCH BACK
      AASAV = AA(4)
      AA(4) = AA(5)
      AA(5) = AASAV
C
C
C
      DO 30 J = 1, 8
      PR(KK,J) = 0.
      DO 29 K = 1, 34
      PRC(KK,J,K) = RR(K)*ISTOI(J,K)
      PR(KK,J) = PR(KK,J) + PRC(KK,J,K)
   29 CONTINUE
      PRTOT(KK,J) = PR(KK,J) + YI(J,1)
      PRTOAB(KK,J) = ABS(PRTOT(KK,J))
```

```
   30 CONTINUE
C
C++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C  TWO-WAY REACTION  PRODUCTION RATES: ----------------------
C
      DO 40 J = 1, 8
      DO 40 KILROY = 1, 17
      KE = KILROY * 2
      KO = KE - 1
      PRC(KK,J,KILROY+34) = PRC(KK,J,KO) + PRC(KK,J,KE)
   40 CONTINUE
C++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C  TWO-WAY REACTION RATES
C
      DO 1010 IFB = 1,17
 1010 RRFB(IFB) = RR(2*IFB-1) - RR(2*IFB)
C
      DO 1020 IFB = 1,17
      IFBMD8 =  IFB/8
      KNSIM = 55 + IFBMD8
      IFBRMD = IFB - (IFB/8)*8
 1020 PRC(KK,IFBRMD,55+IFBMD8) = RRFB(IFB)
C
C  WHEN YOU GOT LEMONS, MAKE LEMONADE:  I WANT TO SEND 17 QUANTITIES
C  INDEPENDENT OF SPECIES THROUGH PRC(100,8,X).  RATHER THAN JUST USE THE
C  FIRST SLOT OUT OF 8 FOR 17 EXTRA IN X, DIVIDE 17 INTO GROUPS OF 8 PLUS
C  A REMAINDER.
C
C++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C
C     WRITE(6,2003) X(KK), DX, NSTEP, KK
C     WRITE(9,2003) X(KK), DX, NSTEP, KK
C     WRITE(6,2001)
C     WRITE(6,2002) (AA(J),J=1,8)
C     WRITE(9,2002) (AA(J),J=1,8)
C     WRITE(6,2001)
C     WRITE(6,2002) (PR(KK,J),J=1,8)
C     WRITE(9,2002) (PR(KK,J),J=1,8)
C     WRITE(6,2002)
C
CCCCCCCCCCCCCCCCC      DO 200 K = 1, 34
CCCCCCCCCCCCCCCCC      KMOD2 = 2*(K/2)
C
CCCCCCCCCCCCCCCCC                          KFB = (K+1)/2
CCCCCCCCCCCCCCCCCC     IF(KMOD2 .EQ. K)    KFB = K/2
CCCCCCCCCCCCCCCCCC     REDUNDANT.
C
CCCCCCCCCCCCCCCCC      WRITE(6,2007) K, KFB, RRC(K), RR(K), (PRC(KK,J,K),J=1,8)
CCCCCCCCCCCCCCCCC      WRITE(9,2007) K, KFB, RRC(K), RR(K), (PRC(KK,J,K),J=1,8)
CCCCCCCCCCCCCCCCC      IF(KMOD2 .EQ. K) WRITE(6,2004)
```

```
CCCCCCCCCCCCCCCCC 200 CONTINUE
C
CCCCCCCCCCCCCCCCC      WRITE(6,2000)
C
 1000 CONTINUE
C
C
 1999 FORMAT(1H1)
 2000 FORMAT(1H )
 1501 FORMAT(1H ,1PE10.3,11E11.3)
 2001 FORMAT(1H )
 2002 FORMAT(1H ,31X,1P8E12.4)
 2003 FORMAT(1H ,31X,1P2E12.4,50X,I7,3X,I3)
 2004 FORMAT(1H )
 2007 FORMAT(1H ,I2,1X,I2,1P2E12.4, 2X , 8E12.4)
      RETURN
      END
-----------------------------
*****************************
-----------------------------
```

CHAPTER VI

```
-------------------------------
            AAB.TW1
-------------------------------
@@DIFKIN JOB (2003,5006,450,20),'PAUL SCHIPPNICK',REGION=512K,
@@ CLASS=1
@*PASSWORD   12,AP
@*ROUTE PRINT LOCAL
@@ EXEC FORTXCG,LPARM=NOMAP
@@SYSPRINT DD DUMMY
@*INCLUDE A.1  20035006,12
@*INCLUDE B.2  20035006,12
@*INCLUDE B.3  20035006,12
@@GO.FT02F001 DD DSN=&&AA,UNIT=VIO,SPACE=(TRK,(1,1),RLSE),DISP=(,PASS),
@@ DCB=(RECFM=VSB,BLKSIZE=1000,LRECL=1000)
@@GO.FT13F001  DD *
@*INCLUDE CHEMRAD  22035001,6
@*INCLUDE ZZ.CHEM+  20035006,12
@*INCLUDE MKREACT  20035006,12
@*INCLUDE COMP81FB  20035006,12
 199 H      +DH      +M      =EXC1   +M                73 3.9E-25 2.  0.
@@GO.SYSIN  DD *
    1M
AS      99
DS      49    66    85    89
AR     199
```

```
DR        1    2    3    4    5    6    7    8

1000.     400.       1.8400E+19 3.670E+14    8.6
EC,TC=0.1TD,TD=1.3E-6,TMIN=TC/100,TMAX=1/BET=1/3067,P=1ATM,N=1.84E19,I=3.67E14
   21    1    0    1    1    1    1
.1        1.         .05             6.5E-8
    1.4E-9.00035          1.E-14
    1
1000.     50.
1.00      20.0       1.00       150.
0.1       21.8       1.92       1.3       0.01      0.02      0.03      675.
0.01      0.02       0.03       0.04      0.05      0.06      0.07      0.08
0.11      0.12       0.13       0.14      0.15      0.16      0.17      0.18
0.21      0.22       0.23       0.24      0.25      0.26      0.27      0.28
    1
0.        1.         .913
@@ EXEC FORTXCG,LPARM='SIZE=512K'
@@SYSPRINT DD DUMMY
C       MAIN PROGRAM FOR BOAT
C
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.MODK  20035006,12
@*INCLUDE B.UT  20035006,12
      SUBROUTINE BOATIC
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.IC.NEU  20035006,12
@*INCLUDE B.PREP  20035006,12
      SUBROUTINE BOATYI
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.YI.HOH  20035006,12
@*INCLUDE A.NR  20035006,12
@*INCLUDE UT.SMBBL  20035006,12
      SUBROUTINE BOATCC (K, I, L, NJ, NEQ, QSIGN, RMFAC)
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.CC  20035006,12
      FUNCTION BOATEF (K, NJ, RRT)
C
C*    BOATEF - CALCULATE E USED IN BOATS2
C
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.EF  20035006,12
      SUBROUTINE BOATS2
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.S2DKED  20035006,12
      SUBROUTINE BOATM1
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.M1DKED 20035006,12
      FUNCTION CHEM ( CAS )
@*INCLUDE ADDDDD 20035006,12
@*INCLUDE B.CHM 20035006,12
```

```
      SUBROUTINE BOATM2
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.M2DKNM  20035006,12
      SUBROUTINE BOATS3 (L)
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.S3DK  20035006,12
      SUBROUTINE BOATGX
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.GXDK  20035006,12
      SUBROUTINE BOATIN
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.INDK  20035006,12
      SUBROUTINE BOATSA
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.SADK  20035006,12
      SUBROUTINE BOATSB
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.SBDKRS  20035006,12
      SUBROUTINE BOATOT
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.OTDKRS  20035006,12
@@GO.FT02F001 DD  DSN=&&AA,DISP=(OLD,DELETE)
@@*
@@GO.FT08F001 DD DSN=UF.B0035006.S1.TW1.T1,UNIT=SYSDA,
@@ DISP=(NEW,CATLG),SPACE=(6072,(100,20),RLSE),
@@ DCB=(RECFM=FB,BLKSIZE=6072,LRECL=132)
@@GO.FT09F001 DD DSN=UF.B0035006.S1.TW1.RS.T1,
@@ DISP=(NEW,CATLG),DCB=(BLKSIZE=6072,LRECL=132,RECFM=FB),
@@ UNIT=SYSDA,SPACE=(TRK,(5,5))
@@*GO.FT08F001 DD DUMMY
@@*GO.FT09F001 DD DUMMY
@@GO.FT10F001 DD DUMMY
@@*GO.FT10F001 DD DSN=UF.B0035006.S1.TW1.RS.T0,
@@* DISP=(OLD,KEEP),DCB=(BLKSIZE=6072,LRECL=132,RECFM=FB),
@@* SPACE=(TRK,(5,5))
@@GO.SYSIN DD *
      H         1.2920
      H2O       0.2502
      OH        0.3695
      EXC1      0.2502
@*INCLUDE YI.1000S  20035006,12
--------------------------------
            AAB.I18
--------------------------------
@@DIFKIN JOB (2003,5006,4000,40,0),'PAUL SCHIPPNICK',REGION=512K,
@@ CLASS=0
@*PASSWORD
@*ROUTE PRINT LOCAL
@@ EXEC FORTXCG,LPARM=NOMAP
@@SYSPRINT DD DUMMY
```

```
@*INCLUDE A.1  20035006,12
@*INCLUDE B.2  20035006,12
@*INCLUDE B.3  20035006,12
@@GO.FT02F001 DD DSN=&&AA,UNIT=VIO,SPACE=(TRK,(1,1),RLSE),DISP=(,PASS),
@@ DCB=(RECFM=VSB,BLKSIZE=1000,LRECL=1000)
@@GO.FT13F001  DD *
@*INCLUDE CHEMRAD  20035006,12
@*INCLUDE ZZ.CHEM+  20035006,12
@*INCLUDE MKREACT  20035006,12
@*INCLUDE COMP81FB  20035006,12
@@GO.SYSIN  DD *
    1M
AS      58   59
DS      66
AR     165  166  167  168  169  170  171  172  173  174  175  176  177  178  179
AR     180  181  182  183  184  185  186  187  188  189  190  191  192  193  194
AR     195  196  197  198
DR       1    2    3    4    5    6    7    8

1000.      400.       6.0000E+15 1.000E+18   8.6
EC,TC=.00208,TD=.004,TMIN=3E-6,TMX=1,BET=1,N=6E15,I=1E18,NEAR DEPLETION BNDRY
   21     1     0     1     1     1     1
.1        1.         .05          1.0E-3
     3.E-61.                1.E-14
    1
1000.      50.
1.00       20.0       1.00       150.
0.1        21.8       1.92       1.3        0.01       0.02       0.03       .242
0.01       0.02       0.03       0.04       0.05       0.06       0.07       0.08
0.11       0.12       0.13       0.14       0.15       0.16       0.17       0.18
0.21       0.22       0.23       0.24       0.25       0.26       0.27       0.28
    1
0.         1.         .913
@@ EXEC FORTXCG,LPARM='SIZE=512K'
@@SYSPRINT DD DUMMY
C       MAIN PROGRAM FOR BOAT
C
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.MOOK  20035006,12
@*INCLUDE B.UT  20035006,12
      SUBROUTINE BOATIC
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.IC.NEU  20035006,12
@*INCLUDE B.PREP  20035006,12
      SUBROUTINE BOATYI
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.YI.NEU  20035006,12
@*INCLUDE A.NR  20035006,12
@*INCLUDE UT.SMSON  20035006,12
      SUBROUTINE BOATCC (K, I, L, NJ, NEQ, QSIGN, RMFAC)
```

```
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.CC  20035006,12
      FUNCTION BOATEF (K, NJ, RRT)
C
C*     BOATEF - CALCULATE E USED IN BOATS2
C
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.EF  20035006,12
      SUBROUTINE BOATS2
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.S2DKED  20035006,12
      SUBROUTINE BOATM1
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.M1DKED 20035006,12
      FUNCTION CHEM ( CAS )
@*INCLUDE ADDDDD 20035006,12
@*INCLUDE B.CHM 20035006,12
      SUBROUTINE BOATM2
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.M2DKNM  20035006,12
      SUBROUTINE BOATS3 (L)
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.S3DK  20035006,12
      SUBROUTINE BOATGX
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.GXDK  20035006,12
      SUBROUTINE BOATIN
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.INDK  20035006,12
      SUBROUTINE BOATSA
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.SADK  20035006,12
      SUBROUTINE BOATSB
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.SBDKRS  20035006,12
      SUBROUTINE BOATOT
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.OTDKRS  20035006,12
@@GO.FT02F001 DD  DSN=&&AA,DISP=(OLD,DELETE)
@@*
@@GO.FT08F001 DD DSN=UF.B0035006.S1.NTCHM.EV1000.I18.T1,UNIT=SYSDA,
@@ DISP=(NEW,CATLG),SPACE=(6072,(100,20),RLSE),
@@ DCB=(RECFM=FB,BLKSIZE=6072,LRECL=132)
@@GO.FT09F001 DD DSN=UF.B0035006.S1.NTCHM.RS.EV1000.I18.T1,
@@ DISP=(NEW,CATLG),DCB=(BLKSIZE=6072,LRECL=132,RECFM=FB),
@@ UNIT=SYSDA,SPACE=(TRK,(5,5))
@@*GO.FT08F001 DD DUMMY
@@*GO.FT09F001 DD DUMMY
@@GO.FT10F001 DD DUMMY
@@*GO.FT10F001 DD DSN=UF.B0035006.S1.NTCHM.RS.EV1000.I18.T0,
```

```
@@* DISP=(OLD,KEEP),DCB=(BLKSIZE=6072,LRECL=132,RECFM=FB),
@@* SPACE=(TRK,(5,5))
@@GO.SYSIN DD *
@*INCLUDE DDD.DFNE  20035006,12
@*INCLUDE YI.1000S  20035006,12
-------------------------------
              AAB.A1C
-------------------------------
@@DIFKIN JOB (2003,5006,4000,40,0),'PAUL SCHIPPNICK',REGION=512K,
@@ CLASS=0
@*PASSWORD
@*ROUTE PRINT LOCAL
@@ EXEC FORTXCG,LPARM=NOMAP
@@SYSPRINT DD DUMMY
@*INCLUDE A.1  20035006,12
@*INCLUDE B.2  20035006,12
@*INCLUDE B.3  20035006,12
@@GO.FT02F001 DD DSN=&&AA,UNIT=VIO,SPACE=(TRK,(1,1),RLSE),DISP=(,PASS),
@@ DCB=(RECFM=VSB,BLKSIZE=1000,LRECL=1000)
@@GO.FT13F001  DD *
@*INCLUDE CHEMRAD  20035006,12
@*INCLUDE ZZ.CHEM+  20035006,12
@*INCLUDE MKREACT  20035006,12
@*INCLUDE COMP81FB  20035006,12
@@GO.SYSIN  DD *
    1M
AS      58    59
DS      66
AR     165   166   167   168   169   170   171   172   173   174   175   176   177   178   179
AR     180   181   182   183   184   185   186   187   188   189   190   191   192   193   194
AR     195   196   197   198
DR       1     2     3     4     5     6     7     8

1000.      400.       1.8400E+19 3.670E+14    8.6
EC,TC=0.1TD,TD=1.3E-6,TMIN=TC@100,TMAX=1@BET=1@3067,P=1ATM,N=1.84E19,I=3.67E14
  21     1     0     1     1     1     1
.1        1.        .05        6.5E-8
    1.4E-9.00035        1.E-14
    1
1000.      50.
1.00       20.0       1.00       150.
0.1        21.8       1.92       1.3        0.01       0.02       0.03       675.
0.01       0.02       0.03       0.04       0.05       0.06       0.07       0.08
0.11       0.12       0.13       0.14       0.15       0.16       0.17       0.18
0.21       0.22       0.23       0.24       0.25       0.26       0.27       0.28
    1
0.         1.         .913
@@ EXEC FORTXCG,LPARM='SIZE=512K'
@@SYSPRINT DD DUMMY
C       MAIN PROGRAM FOR BOAT
```

```
C
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.MODK  20035006,12
@*INCLUDE B.UT  20035006,12
      SUBROUTINE BOATIC
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.IC.NEU  20035006,12
@*INCLUDE B.PREP  20035006,12
      SUBROUTINE BOATYI
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.YI.NEU  20035006,12
@*INCLUDE A.NR  20035006,12
@*INCLUDE UT.SMSON  20035006,12
      SUBROUTINE BOATCC (K, I, L, NJ, NEQ, QSIGN, RMFAC)
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.CC  20035006,12
      FUNCTION BOATEF (K, NJ, RRT)
C
C*    BOATEF - CALCULATE E USED IN BOATS2
C
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.EF  20035006,12
      SUBROUTINE BOATS2
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.S2DKED  20035006,12
      SUBROUTINE BOATM1
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.M1DKED 20035006,12
      FUNCTION CHEM ( CAS )
@*INCLUDE ADDDDD 20035006,12
@*INCLUDE B.CHM 20035006,12
      SUBROUTINE BOATM2
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.M2DKNM  20035006,12
      SUBROUTINE BOATS3 (L)
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.S3DK  20035006,12
      SUBROUTINE BOATGX
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.GXDK  20035006,12
      SUBROUTINE BOATIN
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.INDK  20035006,12
      SUBROUTINE BOATSA
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.SADK  20035006,12
      SUBROUTINE BOATSB
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.SBDKRS  20035006,12
      SUBROUTINE BOATDT
```

```
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.OTDKRS  20035006,12
@@GO.FT02F001 DD  DSN=&&AA,DISP=(OLD,DELETE)
@@*
@@GO.FT08F001 DD DSN=UF.B0035006.S1.NTCHM.EV1000.A1C.T1,UNIT=SYSDA,
@@ DISP=(NEW,CATLG),SPACE=(6072,(100,20),RLSE),
@@ DCB=(RECFM=FB,BLKSIZE=6072,LRECL=132)
@@GO.FT09F001 DD DSN=UF.B0035006.S1.NTCHM.RS.EV1000.A1C.T1,
@@ DISP=(NEW,CATLG),DCB=(BLKSIZE=6072,LRECL=132,RECFM=FB),
@@ UNIT=SYSDA,SPACE=(TRK,(5,5))
@@*GO.FT06F001 DD DUMMY
@@*GO.FT09F001 DD DUMMY
@@GO.FT10F001 DD DUMMY
@@*GO.FT10F001 DD DSN=UF.B0035006.S1.NTCHM.RS.EV1000.A1C.T0,
@@* DISP=(OLD,KEEP),DCB=(BLKSIZE=6072,LRECL=132,RECFM=FB),
@@* SPACE=(TRK,(5,5))
@@GO.SYSIN DD *
@*INCLUDE DDD.DFNE  20035006,12
@*INCLUDE YI.1000S  20035006,12
-------------------------------
              AAB.LIQ1
-------------------------------
@@DIFKIN JOB (2003,5006,4000,40,0),'PAUL SCHIPPNICK',REGION=512K,
@@ CLASS=0
@*PASSWORD
@*ROUTE PRINT LOCAL
@@ EXEC FORTXCG,LPARM=NOMAP
@@SYSPRINT DD DUMMY
@*INCLUDE A.1  20035006,12
@*INCLUDE B.2  20035006,12
@*INCLUDE B.3  20035006,12
@@GO.FT02F001 DD DSN=&&AA,UNIT=VIO,SPACE=(TRK,(1,1),RLSE),DISP=(,PASS),
@@ DCB=(RECFM=VSB,BLKSIZE=1000,LRECL=1000)
@@GO.FT13F001  DD *
@*INCLUDE CHEMRAD  20035006,12
@*INCLUDE ZZ.CHEM+  20035006,12
@*INCLUDE MKREACT  20035006,12
@*INCLUDE COMP81FB  20035006,12
@@GO.SYSIN  DD *
    1M
AS      58   59
DS      66
AR     165  166  167  168  169  170  171  172  173  174  175  176  177  178  179
AR     180  181  182  183  184  185  186  187  188  189  190  191  192  193  194
AR     195  196  197  198
DR       1    2    3    4    5    6    7    8

1000.      300.      3.3400E+22 1.440E+07   8.6
EC TC=.1TD,TD=7.2E-10,TMIN=TC@100,TMAX=1@BET=1.8E-7,E0=1KEV,T=300,N=3LIQ,I=1.44E
   21    1    0    1    1    1    1
```

```
.1          1.          .05          3.6E-11
   7.2E-13     1.8E-7     1.E-14
     1
1000.       50.
1.00        20.0        1.00        150.
0.1         21.8        1.92        1.3         0.01        0.02        0.03        1.35E6
0.01        0.02        0.03        0.04        0.05        0.06        0.07        0.08
0.11        0.12        0.13        0.14        0.15        0.16        0.17        0.18
0.21        0.22        0.23        0.24        0.25        0.26        0.27        0.28
     1
0.          1.          .913
@@ EXEC FORTXCG,LPARM='SIZE=512K'
@@SYSPRINT DD DUMMY
C       MAIN PROGRAM FOR BOAT
C
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.MODK  20035006,12
@*INCLUDE B.UT  20035006,12
      SUBROUTINE BOATIC
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.IC.NEU  20035006,12
@*INCLUDE B.PREP  20035006,12
      SUBROUTINE BOATYI
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.YI.NEU  20035006,12
@*INCLUDE A.NR  20035006,12
@*INCLUDE UT.SMSON  20035006,12
      SUBROUTINE BOATCC (K, I, L, NJ, NEQ, QSIGN, RMFAC)
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.CC  20035006,12
      FUNCTION BOATEF (K, NJ, RRT)
C
C*     BOATEF - CALCULATE E USED IN BOATS2
C
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.EF  20035006,12
      SUBROUTINE BOATS2
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.S2DKED  20035006,12
      SUBROUTINE BOATM1
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.M1DKED 20035006,12
      FUNCTION CHEM ( CAS )
@*INCLUDE ADDDDD 20035006,12
@*INCLUDE B.CHM 20035006,12
      SUBROUTINE BOATM2
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.M2DKNM  20035006,12
      SUBROUTINE BOATS3 (L)
@*INCLUDE ADDDDD  20035006,12
```

```
@*INCLUDE B.S3DK  20035006,12
      SUBROUTINE BOATGX
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.GXDK  20035006,12
      SUBROUTINE BOATIN
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.INDK  20035006,12
      SUBROUTINE BOATSA
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.SADK  20035006,12
      SUBROUTINE BOATSB
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE A.SBDKRS  20035006,12
      SUBROUTINE BOATOT
@*INCLUDE ADDDDD  20035006,12
@*INCLUDE B.OTDKRS  20035006,12
@@GO.FT02F001 DD  DSN=&&AA,DISP=(OLD,DELETE)
@@*
@@GO.FT08F001 DD DSN=UF.B0035006.S1.NTCHM.EV1000.LIQ1.T1,UNIT=SYSDA,
@@ DISP=(NEW,CATLG),SPACE=(6072,(100,20),RLSE),
@@ DCB=(RECFM=FB,BLKSIZE=6072,LRECL=132)
@@GO.FT09F001 DD DSN=JF.B0035006.S1.NTCHM.RS.EV1000.LIQ1.T1,
@@ DISP=(NEW,CATLG),DCB=(BLKSIZE=6072,LRECL=132,RECFM=FB),
@@ UNIT=SYSDA,SPACE=(TRK,(5,5))
@@*GO.FT08F001 DD DUMMY
@@*GO.FT09F001 DD DUMMY
@@GO.FT10F001 DD DUMMY
@@*GO.FT10F001 DD DSN=UF.B0035006.S1.NTCHM.RS.EV1000.LIQ1.T0,
@@* DISP=(OLD,KEEP),DCB=(BLKSIZE=6072,LRECL=132,RECFM=FB),
@@* SPACE=(TRK,(5,5))
@@GO.SYSIN DD *
@*INCLUDE DDD.DFNE  20035006,12
@*INCLUDE YI.1000S  20035006,12
-------------------------------
                A.1
-------------------------------
C=====================================================================
C=====================================================================
C
C       PROGRAM PROCES
C
C       DATA PROCESSOR FOR BOAT CODE.  READS INPUT DATA
C       AND CREATES INPUT DATA FILES FOR RUNNING BOAT.
C
C=====================================================================
C=====================================================================
C
C=====================================================================
C       PROCESSOR COMMON BLOCK
C=====================================================================
```

```
      REAL MOLWT
C
      COMMON ISYS, NS, NR, WMIX, ALPHAJ(25)
      COMMON LUNIN, LUNOT, NSMAX, NRMAX
      COMMON H298(25), MOLWT(25), SPECID(25), COEF(14,25)
      COMMON AL(25), BL(25), CL(25), SL(25), SH(25), ALL(3)
      COMMON ZID(5,80), IRR(80), IRT(80), RC(80,3)
C
C
C
C        COMMON / SYSTEM / ISYSTM(25+80+2,7)
C
      COMMON / SYSTEM / ISYSTM(107,7)
C
      DIMENSION  TITLE(18), XCHANG(20), PRNTXC(20)
C
C-----------------------------------------------------------------------
      DIMENSION YR(101), ALPHA(25,101), WTMIX(101)
C-----------------------------------------------------------------------
C
C
C================================
C        FIXED INPUT DATA FOR BOAT %
C================================
C
      DATA FDL / 1. /
      DATA LUNBT / 2 /
      DATA SYSM / 4HM     /, NEWSYS / 7 /
C
C=====================================================
C        READ SYSTEM.
C
C.......................................
      LUNIN = 5
      LUNOT = 6
      NSMAX = 25
      NRMAX = 80
      READ (LUNIN,1010) ISYS, SYS
C
      IF ( ISYS .EQ. 0 ) GO TO 100
C
C==============================================
C        CHECK IF SYSTEM CHOSEN IS TO BE MODIFIED
C        OR IF A NEW SYSTEM IS TO BE DEFINED.
C
      IF ( (SYS.EQ.SYSM) .OR. (ISYS.EQ.NEWSYS) ) CALL SYSMOD
C
C==============================================
C        ACCESS DATA BANK FOR SPECIES AND THERMO DATA
C
            CALL DABANK
```

```
C=================================================
C
C.........................................
  100 READ (LUNIN,2000) E0, T, DENS, RATE, Z0
C
C
C*********************************************************************
C************************
C
C        BOAT INPUT
C
C************************
C*********************************************************************
C
C=========================================================
C        ACCESS DATA BANK FOR LOW TEMPERATURE COEFFICIENTS
C        FOR BOAT.
C
  550        CALL LOCOB
C=========================================================
C
C.............................................................
      READ (LUNIN,8000) TITLE
      WRITE(LUNBT,8000) TITLE
C.............................................................
      READ(LUNIN,1000) MPSI, ICHM, IOUT1,IOUT2,IOUT3,IOUT4,IOUT5
     $,IOUT6
      IF ( ICHM .EQ. 0 ) NR = 0
C
      WRITE(LUNBT,1000) MPSI, NS, NR, IOUT1,IOUT2,IOUT3,IOUT4,
     $IOUT5,IOUT6
C
C.........................................................
      READ(LUNIN,2000) CPR, XIO, CINT, CCHM
      WRITE(LUNBT,2222) CPR, XIO, CINT, CCHM
      WRITE(6,2228) CPR, XIO, CINT, CCHM
 2228 FORMAT(1H0, 'CPR, XIO, CINT, CCHM = ', 1P4E11.4)
C.........................................................
C
  700 READ (LUNIN,2000) X, XMAX, PRNT, DXMIN
      WRITE(LUNBT,2222) X, XMAX, PRNT, FDL, DXMIN
C
      READ(LUNIN,1000) NXC
      WRITE(LUNBT,1000) NXC
C
      READ(LUNIN,2000) (XCHANG(I),PRNTXC(I), I=1,NXC)
      WRITE(LUNBT,2222) (XCHANG(I),PRNTXC(I), I=1,NXC)
C
C.........................................
      WRITE(LUNBT,2222) E0, T, DENS, RATE, Z0
```

```
C.....................................................................
C
C
      READ(LUNIN,2000) BBO, XIB, PB, XIEDGE
      WRITE(LUNBT,2222) BBO, XIB, PB, XIEDGE
      WRITE(6,2223) BBO,XIB,PB, XIEDGE
 2223 FORMAT(1H0,'BBO, XIB, PB,  XIEDGE = ',1P4E11.4)
C
C
C.....................................................................
C
C  READ IN PARAMETER VECTOR PXIO AND THREE OTHER USEFUL PARAMETER VECTORS
C  IN CASE THE NEED ARISES  HERE IS SPACE
C
      READ(LUNIN,2000) (YR(I), I = 1, 8)
      WRITE(LUNBT,2222) (YR(I), I = 1, 8)
      WRITE(6,2224)
      WRITE(6,2222) (YR(I), I = 1, 8)
C
C
      READ(LUNIN,2000) (YR(I), I = 1, 8)
      WRITE(LUNBT,2222) (YR(I), I = 1, 8)
      WRITE(6,2225)
      WRITE(6,2222) (YR(I), I = 1, 8)
C
C
      READ(LUNIN,2000) (YR(I), I = 1, 8)
      WRITE(LUNBT,2222) (YR(I), I = 1, 8)
      WRITE(6,2226)
      WRITE(6,2222) (YR(I), I = 1, 8)
C
C
      READ(LUNIN,2000) (YR(I), I = 1, 8)
      WRITE(LUNBT,2222) (YR(I), I = 1, 8)
      WRITE(6,2227)
      WRITE(6,2222) (YR(I), I = 1, 8)
C
C
 2224 FORMAT(1H0,'PXIO')
 2225 FORMAT(1H0,'PXX1')
 2226 FORMAT(1H0,'PXX2')
 2227 FORMAT(1H0,'PXX3')
C
C
C.....................................................................
C  READ IN ETA GRID ARRAY
C
C
C
      READ(LUNIN,1000) NET
```

```
C
C
 1500 CONTINUE
C
C=========================================
C        FORMAT STATEMENTS %
C=========================================
C
 1000 FORMAT ( 16I5 )
C
C1010 FORMAT ( 2I5, A1 )
 1010 FORMAT (  I5, A1 )
C
 1111 FORMAT ( I1, 1X, 4( A4,2X ), F10.3 )
 2000 FORMAT ( 8E10.5 )
 2222 FORMAT ( 8E10.5 )
C2222 FORMAT ( 8(1PE10.3) )
 3000 FORMAT ( F10.3, 4( A4,2X ), A4 )
 3333 FORMAT ( 5(1PD15.7) )
 4000 FORMAT ( 3A2, 1X, 3A2, 1X, 2F10.3, 16X, A4 )
 4444 FORMAT(I1,1X,3A2,1X,3A2,1X,2F10.0,1X,I1)
 5000 FORMAT ( 20A4 )
 6000 FORMAT ( A4, 1X, 2(1PE10.3) )
 7000 FORMAT ( A4, 3X, A4, 10X, A4, 3X, A4, 3X, A4, 9X, I2, I1,
     #         E8.2, F4.1, F9.1 )
 7010 FORMAT(20A4)
 8000 FORMAT ( 18A4, A4 )
 9000 FORMAT ( 6(1PE13.6) )
C
      STOP
      END
      SUBROUTINE SYSMOD
C=========================================================
C        CHEMICAL SYSTEMS MODIFICATION ROUTINE %
C
C        ADD TO/DELETE SPECIES AND CHEMICAL REACTIONS
C        FROM ANY OF THE EXISTING SPECIFIED CHEMICAL
C        SYSTEMS, OR SPECIFY A NEW SYSTEM FROM THE
C        AVAILABLE SPECIES AND REACTIONS ON THE DATA BANK.
C=========================================================
C
C=================================================================
C        PROCESSOR COMMON BLOCK
C=================================================================
      REAL MOLWT
C
      COMMON ISYS, NS, NR, WMIX, ALPHAJ(25)
      COMMON LUNIN, LUNOT, NSMAX, NRMAX
      COMMON H298(25), MOLWT(25), SPECID(25), COEF(14,25)
      COMMON AL(25), BL(25), CL(25), SL(25), SH(25), ALL(3)
```

```
      COMMON ZID(5,80), IRR(80), IRT(80), RC(80,3)
C
C
C***     PDP ONLY ...
C        COMMON / SYSTEM / ISYSTM(25+80+2,7)
C***     END PDP
C***     CDC ONLY ...
      COMMON / SYSTEM / ISYSTM(107,7)
C***     END CDC
C
C        END
C
      DIMENSION MTYPE(7), MODNUM(15), ISMOD(80), RCNEW(80)
C***     PDP ONLY ...
C        DIMENSION ISBLD(25+1), IRBLD(80+1)
C***     END PDP
C***     CDC ONLY ...
      DIMENSION ISBLD(26),    IRBLD(81)
C***     END CDC
C
      DATA MTYPE / 2HAS, 2HDS, 2HAR, 2HDR, 2HSS, 2HSR, 2H   /
C
C=========================================================
C        MOVE SPECIES AND REACTION NUMBERS INTO THE TEMPORARY
C        BUILD VECTORS ISBLD AND IRBLD.
C
      CALL SIVMV (ISYSTM(1,ISYS), ISBLD, ISYSTM(1,ISYS)+1)
      CALL SIVMV (ISYSTM(ISYSTM(1,ISYS)+2,ISYS), IRBLD,
     #            ISYSTM(ISYSTM(1,ISYS)+2,ISYS)+1)
C
C=================================================
C        READ MODIFICATION CARDS AND DETERMINE TYPE.
C
C.................................................
  100 READ (LUNIN,2000) MODTYP, (MODNUM(J), J=1,15)
C
      DO 200  J=1,7
         IF ( MODTYP .EQ. MTYPE(J) ) GO TO 300
  200 CONTINUE
      WRITE(LUNOT,4000)
      STOP
C
  300 GO TO ( 400, 400, 400, 400, 500, 500, 1200 ) , J
C
  400 NS = ISBLD(1)
      NR = IRBLD(1)
C
  500 GO TO ( 600, 700, 800, 900, 1000, 1100, 1200 ) , J
C
C
```

```
C==============================
C        ADD SPECIES TO A SYSTEM
C
  600 IM = 1
      IS = 0
      DO 630  J=1,NS
  610     IS = IS + 1
          IF ( (MODNUM(IM).LT.ISBLD(J+1)) .AND.
     #         (MODNUM(IM).NE.0)  ) GO TO 620
          ISMOD(IS) = ISBLD(J+1)
          IF ( IS .GE. NSMAX  ) GO TO 650
          IF ( (MODNUM(IM).GT.ISBLD(NS)) .AND.
     #         (J.EQ.NS) ) GO TO 640
          GO TO 630
  620     ISMOD(IS) = MODNUM(IM)
          IF ( IS .GE. NSMAX  ) GO TO 650
          IM = IM + 1
          IF ( (MODNUM(IM).GT.ISBLD(NS)) .AND.
     #         (J.EQ.NS) ) GO TO 640
          GO TO 610
  630 CONTINUE
      GO TO 650
  640 IS = IS + 1
      ISMOD(IS) = MODNUM(IM)
      IF ( IS .GE. NSMAX ) GO TO 650
      IM = IM + 1
      IF ( MODNUM(IM) .EQ. 0 ) GO TO 650
      GO TO 640
  650 ISBLD(1) = IS
      CALL SIVMV (ISMOD, ISBLD(2), IS)
      GO TO 100
C
C==================================
C        DELETE SPECIES FROM A SYSTEM
C
  700 IM = 1
      IS = 0
      DO 720  J=1,NS
          IS = IS + 1
          IF ( MODNUM(IM) .EQ. ISBLD(J+1) ) GO TO 710
          ISMOD(IS) = ISBLD(J+1)
          GO TO 720
  710     IM = IM + 1
          IS = IS - 1
  720 CONTINUE
      ISBLD(1) = IS
      CALL SIVMV (ISMOD, ISBLD(2), IS)
      GO TO 100
C
C==============================
```

```
C        ADD REACTIONS TO A SYSTEM
C
  800 IM = 1
      IS = 0
      DO 830  J=1,NR
  810     IS = IS + 1
          IF ( (MODNUM(IM).LT.IRBLD(J+1)) .AND.
     #         (MODNUM(IM).NE.0) ) GO TO 820
          ISMOD(IS) = IRBLD(J+1)
          IF ( IS .GE. NRMAX ) GO TO 850
          IF ( (MODNUM(IM).GT.IRBLD(NR)) .AND.
     #         (J.EQ.NR) ) GO TO 840
          GO TO 830
  820     ISMOD(IS) = MODNUM(IM)
          IF ( IS .GE. NRMAX ) GO TO 850
          IM = IM + 1
          IF ( (MODNUM(IM).GT.IRBLD(NR)) .AND.
     #         (J.EQ.NR) ) GO TO 840
          GO TO 810
  830 CONTINUE
      GO TO 850
  840 IS = IS + 1
      ISMOD(IS) = MODNUM(IM)
      IF ( IS .GE. NRMAX ) GO TO 850
      IM = IM + 1
      IF ( MODNUM(IM) .EQ. 0 ) GO TO 850
      GO TO 840
  850 IRBLD(1) = IS
      CALL SIVMV (ISMOD, IRBLD(2), IS)
      GO TO 100
C
C=====================================
C        DELETE REACTIONS FROM A SYSTEM
C
  900 IM = 1
      IS = 0
      DO 920  J=1,NR
          IS = IS + 1
```



```
          IF ( MODNUM(IM) .EQ. IRBLD(J+1) ) GO TO 910
          ISMOD(IS) = IRBLD(J+1)
          GO TO 920
  910     IM = IM + 1
          IS = IS - 1
  920 CONTINUE
      IRBLD(1) = IS
      CALL SIVMV (ISMOD, IRBLD(2), IS)
      GO TO 100
```

```
C
C==========================================
C        SPECIFY SPECIES - USER DEFINED SYSTEM
C        SPECIES NUMBERS IN ASCENDING ORDER.
C
 1000 DO 1010  J=1,15
          IF ( (MODNUM(J).EQ.0) .OR. (ISS.GE.NSMAX) ) GO TO 1020
          ISS = ISS + 1
          ISMOD(ISS) = MODNUM(J)
 1010 CONTINUE
 1020 ISBLD(1) = ISS
      CALL SIVMV (ISMOD, ISBLD(2), ISS)
      GO TO 100
C
C==========================================
C        SPECIFY REACTIONS - USER DEFINED SYSTEM
C        REACTION NUMBERS IN ASCENDING ORDER.
C
 1100 DO 1110  J=1,15
          IF ( (MODNUM(J).EQ.0) .OR. (ISR.GE.NRMAX) ) GO TO 1120
          ISR = ISR + 1
          ISMOD(ISR) = MODNUM(J)
 1110 CONTINUE
 1120 IRBLD(1) = ISR
      CALL SIVMV (ISMOD, IRBLD(2), ISR)
      GO TO 100
C
C==========================================================
C        FINISH UP BY MOVING NEWLY BUILT SPECIES AND REACTION
C        NUMBER VECTORS BACK INTO ISYSTM ARRAY.
C
 1200 CALL SIVMV (ISBLD, ISYSTM(1,ISYS), ISBLD(1)+1)
      CALL SIVMV (IRBLD, ISYSTM(ISBLD(1)+2,ISYS), IRBLD(1)+1)
C
      RETURN
C
C*********************************************************************
C**********************
C        ENTRY RRMOD - CHANGE REACTION RATES FOR SPECIFIED
C                      REACTION NUMBERS.
C
C**********************
C*********************************************************************
C
      ENTRY RRMOD
C
C==============================================================
C        CHANGE THE EXISTING REACTION RATES (FROM DATA BANK) FOR THE
C        REACTION NUMBERS SPECIFIED.  REACTION NUMBERS IN ASCENDING
C        ORDER.  A MAXIMUM OF 80 REACTION RATES (5 PER CARD) MAY BE
```

```
C        MODIFIED.
C
      DO 1300  J=1,NRMAX,5
C.....................................................................
C        READ (LUNIN,3000, END=1400) (MODNUM(I), RCNEW(I), I=J,J+4)
       J1=J+4
      READ(LUNIN,3000,END=1400) (MODNUM(I), RCNEW(I), I=J,J1)
 1300 CONTINUE
 1400 IM = 1
      DO 1600  J=1,NR
         IF ( MODNUM(IM) .EQ. 0 ) GO TO 1700
         IF ( MODNUM(IM) .EQ. ISYSTM(ISYSTM(1,ISYS)+2+J,ISYS) )
     #          GO TO 1500
         GO TO 1600
 1500    RC(J,1) = RCNEW(IM)
         IM = IM + 1
 1600 CONTINUE
C
 1700 RETURN
C
C=========================
C        FORMAT STATEMENTS %
C
 2000 FORMAT ( A2, 3X, 15I5 )
 3000 FORMAT ( 5( I3, 2X, E10.4 ) )
 4000 FORMAT ( // 42H *** ERROR ON SYSTEM MODIFICATION CARD *** )
C
      END
      SUBROUTINE SIVMV (VEC1, VEC2, NW)
      DIMENSION VEC1(1), VEC2(1)
C
C     SFVMV - STANDARD FORTRAN VECTOR MOVE
C
      DO 10 I = 1, NW
      VEC2(I) = VEC1(I)
 10   CONTINUE
C
      RETURN
      END
      BLOCK DATA
C
C       COMMON / SYSTEM / ISYSTM(25+80+2,7)
      COMMON / SYSTEM / ISYSTM(107,7)
C
C=====================================================================
C        THIS BLOCK DATA INITIALIZES THE SPECIES AND REACTION
C        NUMBERS TO BE READ IN FOR EACH SPECIFIED SYSTEM.
C        THE SECOND SUBSCRIPT IN THE ARRAY ISYSTM(I,J) DENOTES
C        THE SYSTEM NUMBER.  THE FIRST VALUE OF THIS ARRAY
C        DENOTES THE NUMBER OF SPECIES (NS) IN THE SYSTEM.
```

```
C       THE FOLLOWING NS VALUES ARE THE SPECIES IDENTIFICATION
C       NUMBERS FOR THAT SYSTEM.  THE NEXT VALUE OF THIS ARRAY
C       IS THE NUMBER OF REACTIONS (NR) IN THE SYSTEM FOLLOWED
C       BY NR REACTION IDENTIFICATION NUMBERS FOR THAT SYSTEM.
C       THE DIMENSIONS OF THE ARRAY ISYSTM NOW ACCOMODATE A
C       MAXIMUM OF 25 SPECIES/SYSTEM AND A MAXIMUM OF 80
C       REACTIONS/SYSTEM FOR 7 SYSTEMS.
C
C       THERE ARE PRESENTLY SIX FIXED SYSTEMS DEFINED.  THEY ARE
C       DESCRIBED BELOW.  IF NEW SYSTEMS ARE TO BE ADDED, PUT THE
C       SPECIES AND REACTION IDENTIFICATION NUMBERS IN ASCENDING
C       ORDER.
C
C       SYSTEM %
C
C       01 % HYDROGEN / OXYGEN
C       02 % CARBON   / HYDROGEN / OXYGEN
C       03 % CARBON   / HYDROGEN / OXYGEN   / CHLORINE
C       04 % CARBON   / HYDROGEN / OXYGEN   / CHLORINE / FLUORINE
C       05 % HYDROGEN / OXYGEN   / BORON
C       06 % HYDROGEN / OXYGEN   / BORON    / CHLORINE / FLUORINE
C       07 % USER DEFINED SYSTEM
C
C=====================================================================
      DATA ISYSTM /
     107,  48,49,50,66,85,87,89,  08,  1,2,3,4,5,6,7,8, 90*0,
     209,  29,30,48,49,50,66,85,87,89,  10,  1,2,3,4,5,6,7,8,9,10,
     2  86*0,
     313,  1,29,30,35,39,48,49,50,54,66,85,87,89,  16,  1,2,3,4,5,6,
     37,8,9,10,11,12,13,14,15,16, 76*0,
     415,  29,30,35,39,42,46,48,49,50,54,56,66,85,87,89,  22,  1,2,
     43,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22, 68*0,
     511,  11,15,19,48,49,50,52,66,85,87,89,  16,  1,2,3,4,5,6,7,8,
     523,24,25,26,27,28,29,30, 78*0,
     624,  7,8,9,11,12,13,15,19,29,30,35,39,42,46,48,49,50,52,54,56,
     666,85,87,89,  36,  1,2,3,4,5,7,8,11,12,13,14,17,18,19,20,23,
     624,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,
     645*0,
     7107*0                                                          /
C
C
C     RETURN
      END
      SUBROUTINE DABANK
C==================================================
C       RETRIEVES CHEMICAL SPECIES, THERMO DATA, AND
C       CHEMICAL REACTIONS FOR SPECIFIED SYSTEM.
C==================================================
C
C
```

```
C=====================================================================
C        PROCESSOR COMMON BLOCK
C=====================================================================
      REAL MOLWT
C
      COMMON ISYS, NS, NR, WMIX, ALPHAJ(25)
      COMMON LUNIN, LUNOT, NSMAX, NRMAX
      COMMON H298(25), MDLWT(25), SPECID(25), COEF(14,25)
      COMMON AL(25), BL(25), CL(25), SL(25), SH(25), ALL(3)
      COMMON ZID(5,80), IRR(80), IRT(80), RC(80,3)
C
C
C        COMMON / SYSTEM / ISYSTM(25+80+2,7)
      COMMON / SYSTEM / ISYSTM(107,7)
C
C        END
C
      DATA LUNDB / 13 /,  TX / 300. /,  R / 1.98718 /
      DATA FACTR / 1. /
C
C  CGS-CAL UNITS  * * * * * * * *
      DATA ENDSPC / 4HEND  /
C
      RFACTR = R * FACTR
C
C
C=================================================================
C        RETRIEVE CHEMICAL SPECIES AND CORRESPONDING THERMODYNAMIC
C        DATA ( MOLECULAR WEIGHTS, H298, AND HIGH AND LOW TEMPERATURE
C        RANGE CURVE FIT COEFFICIENTS )
C=================================================================
      IZ = 0
      NS = ISYSTM(1,ISYS)
      NR = ISYSTM(ISYSTM(1,ISYS)+2,ISYS)
C
      DO 100  I=1,NS
              ISKIP = ISYSTM(I+1,ISYS) - IZ*ISYSTM(I,ISYS)
              IZ = 1
      DO 100  J=1,ISKIP
              READ (LUNDB,1000) SPECID(I), MOLWT(I), H298(I),
     #                          (COEF(K,I), K=1,14)
  100 CONTINUE
      RETURN
C*********************************************************************
C**********************
C
C        ENTRY LOCDB - BOAT LOW TEMPERATURE COEFFICIENTS
C
C**********************
C*********************************************************************
```

```
C
      ENTRY LOCOB
C
C=============================================================
C        COMPUTE LOW TEMPERATURE ( LT 300 DEG K ) COEFFICIENTS
C        FOR BOAT.
C=============================================================
      DO 500  J=1,NS
              AL(J) = H298(J)*1000.*FACTR
              H300  = COEF(8,J) + COEF(9,J)*TX/2. + COEF(10,J)*
     #                 TX**2/3. + COEF(11,J)*TX**3/4. + COEF(12,J)*
     #                TX**4/5. + COEF(13,J)/TX
              H300  = H300*RFACTR*TX
              CP300 = COEF(8,J) + COEF(9,J)*TX +COEF(10,J)*TX**2 +
     #                 COEF(11,J)*TX**3 + COEF(12,J)*TX**4
              CP300 = CP300*RFACTR
              BL(J) = ( 2.*H300 - CP300*TX - 2.*AL(J) )/TX
              CL(J) = ( CP300 - BL(J) )/( 2.*TX )
C
  500 CONTINUE
C
      RETURN
C*********************************************************************
C**********************
C
C        ENTRY REACT - BOAT CHEMICAL REACTIONS
C
C**********************
C*********************************************************************
C
      ENTRY REACT
C
C=================================================
C        RETRIEVE CHEMICAL REACTIONS FOR SPECIFIED SYSTEM
C        ( POSITION FILE TO BEGINNING OF REACTIONS )
C=================================================
  700 READ (LUNDB,1010) ENDTST
      IF (ENDTST .NE. ENDSPC)  GO TO 700
C
C
  800 IZ = 0
C
      DO 900  I=1,NR
              ISKIP = ISYSTM(I+1+NS+1,ISYS) - IZ*ISYSTM(I+NS+1,ISYS)
              IZ = 1
      DO 900  J=1,ISKIP
C-------------------------------------------------------------------
C
C   TO ALLOW CORRECT READ-IN OF REACTION TYPES 3 AND 8  --  PFS
C
```

```
      #          READ (LUNDB,2000) (ZID(K,I), K=1,5), HID, IRR(I), IRT(I),
                                   (RC(I,K), K=1,3)
                 IF(IRR(I).NE.3.AND.IRR(I).NE.8) GO TO 3000
                 ZID(3,I)=ZID(4,I)
                 ZID(4,I)=ZID(5,I)
                 ZID(5,I)=HID
 3000 CONTINUE
C-----------------------------------------------------------------------
  900 CONTINUE
C
C
C        FORMAT STATEMENTS %
C
 1000 FORMAT(5X,A4,4X,4X,F10.5,4X,E15.7/(1X,5E15.8))
 1010 FORMAT ( A4)
C2000 FORMAT ( 5X, A4, 3X, A4, 3X, A4, 3X, A4, 3X, A4, 11X, I2, I1,
C     #        E8.2, F4.1, F9.1 )
 2000 FORMAT ( 5X, A4, 3X, A4, 3X, A4, 3X, A4, 3X, A4, 3X,A4,4X,
      #         I2, I1,
      #         E8.2, F4.1, F9.1 )
C
C
      RETURN
      END
-----------------------------
            CHEMRAD
COMMENT:  THIS LIST WAS ADDED TO BY THE AUTHOR ON BASIS OF DATA
OBTAINED FROM SUPPLEMENTS TO JANNAF TABLES (CHASE ET AL., 1974.
J. PHYS. CHEM. REF. DATA, 3:2; 1975. 4:1; 1982. 11:3)
FOR H+, OH+ AND H3O+, AND FROM
GLUSHKO, GURVICH, BERGMAN, VEIJTS, MEDVEDEV, KHATSKURUZOV AND
JUNGMAN, 1978. TERMODINAMICHESKIJE SVOJSTVA INDIVIDUAL'NYKH
VESHCHESTV, MOSKVA: IZDATEL'STVO "NAUKA" FOR H2O+.

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  1  AL203(S)       101.96000       -0.4027940E+03
  0.12065894D+02 0.31581315D-02 0.40988679D-06-0.80395623D-09 0.17762274D-12
 -0.20578231D+06-0.64814160D+02-0.23576695D+01 0.60831625D-01-0.85195037D-04
  0.54358136D-07-0.12629468D-10-0.20288962D+06 0.47636687D+01
  2  AL203(L)       101.96000        0.3733560E+03
  0.20129179D+02 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00
 -0.20365244D+06-0.11488425D+03 0.00000000D+00 0.00000000D+00 0.00000000D+00
  0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00
  3  BCL             46.27700        0.3168200E+02
  0.41020571D+01 0.48659193D-03-0.18864326D-06 0.35833342D-10-0.25099069D-14
  0.15687958D+05 0.19420655D+01 0.28364463D+01 0.44368812D-02-0.43887522D-05
  0.15161078D-08 0.32646195D-13 0.16001361D+05 0.83321464D+01
  4  BCLF            65.27700       -0.7763100E+02
  0.57076757D+01 0.14100203D-02-0.60114137D-06 0.11367044D-09-0.79368063D-14
 -0.39693327D+05-0.15482176D+01 0.33120234D+01 0.74198763D-02-0.43485949D-05
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-0.11374057D-08 0.13763890D-11-0.39017548D+05 0.10935177D+02
 5  BCL2          81.73400      -0.2277500E+02
 0.64459838D+01 0.57927948D-03-0.26049705D-06 0.63596358D-10-0.53982215D-14
-0.11661304D+05-0.44740401D+01 0.32974785D+01 0.12082576D-01-0.16123755D-04
 0.96265856D-08-0.20599199D-11-0.10956537D+05 0.11029363D+02
 6  BCL3         117.19100      -0.9966100E+02
 0.85985380D+01 0.15531923D-02-0.67000602D-06 0.12789112D-09-0.90000059D-14
-0.51357071D+05-0.15171594D+02 0.37395265D+01 0.18105813D-01-0.21340461D-04
 0.10828335D-07-0.17325967D-11-0.50214609D+05 0.90399632D+01
 7  BF           29.82000      -0.2977800E+02
 0.35771888D+01 0.10192908D-02-0.41251564D-06 0.77196438D-10-0.53498741D-14
-0.15127264D+05 0.32529088D+01 0.34613609D+01-0.95685468D-03 0.60135744D-05
-0.64978057D-08 0.22355349D-11-0.14969820D+05 0.44475660D+01
 8  BF2          48.82000      -0.1325430E+03
 0.54447457D+01 0.17533211D-02-0.78444474D-06 0.15719859D-09-0.11311071D-13
-0.72860367D+05-0.22865127D+01 0.30309303D+01 0.72411021D-02-0.28250919D-05
-0.28920413D-08 0.20046102D-11-0.72151102D+05 0.10432510D+02
 9  BF3          67.80620      -0.2668536E+03
 0.70241985D+01 0.32221559D-02-0.13705154D-05 0.25919671D-09-0.18123110D-13
-0.13918072D+06-0.11197486D+02 0.24468244D+01 0.15276312D-01-0.10784617D-04
 0.68907502D-09 0.14893187D-11-0.13790135D+06 0.12554636D+02
10  BN(S)        24.81770      -0.6059800E+02
 0.90909293D+00 0.81143277D-02-0.48032086D-05 0.12291916D-08-0.11517125D-12
-0.30858565D+05-0.58284487D+01-0.11182452D+01 0.15038275D-01-0.11887860D-04
 0.21058502D-08 0.11962119D-11-0.30413091D+05 0.41742190D+01
11  BO           26.81040      -0.2073000E+01
 0.31564956D+01 0.13816589D-02-0.55049630D-06 0.99116678D-10-0.64164546D-14
-0.10303422D+04 0.60242706D+01 0.37297250D+01-0.20878324D-02 0.57362849D-05
-0.43894828D-08 0.10916632D-11-0.10618859D+04 0.36123221D+01
12  BOCL         62.27700      -0.7813600E+02
 0.57135566D+01 0.18646489D-02-0.77487898D-06 0.14398572D-09-0.99317745D-14
-0.39977353D+05-0.48935834D+01 0.32705321D+01 0.10227750D-01-0.12070163D-04
 0.72025562D-08-0.16914738D-11-0.39378208D+05 0.73361224D+01
13  BOF          45.82000      -0.1463740E+03
 0.52618488D+01 0.23462431D-02-0.97620810D-06 0.18167625D-09-0.12545891D-13
-0.74324949D+05-0.40591029D+01 0.27741485D+01 0.93927631D-02-0.79998507D-05
 0.27457058D-08-0.11175219D-12-0.73640460D+05 0.87507490D+01
14  BOF2         64.80720      -0.2027570E+03
 0.73077233D+01 0.29903620D-02-0.13059617D-05 0.25308242D-09-0.17687333D-13
-0.10334576D+06-0.11205602D+02 0.17445977D+01 0.18693277D-01-0.15246164D-04
 0.26559470D-08 0.13798606D-11-0.10186758D+06 0.17339953D+02
15  BO2          42.80980      -0.7056500E+02
 0.58198434D+01 0.18626574D-02-0.81302797D-06 0.15735821D-09-0.10944238D-13
-0.36255117D+05-0.65741060D+01 0.31212048D+01 0.84680883D-02-0.45972278D-05
-0.16420021D-08 0.16658233D-11-0.35483307D+05 0.75346936D+01
16  BO2-         42.81035      -0.1660000E+03
 0.48805169D+01 0.26743651D-02-0.10932194D-05 0.20080873D-09-0.13717769D-13
-0.85284324D+05-0.30224936D+01 0.24916337D+01 0.97470644D-02-0.87640864D-05
 0.35802544D-08-0.40611221D-12-0.84641218D+05 0.92136785D+01
17  B202         53.64000      -0.1119630E+03
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-0.57296178D+05-0.12180996D+02 0.36870778D+01 0.15361132D-01-0.18606097D-04
 0.12171451D-07-0.32411018D-11-0.56486647D+05 0.43429084D+01
18  B203(L)          69.64000          -0.2992800E+03
 0.15600114D+02 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00
-0.15684455D+06-0.83126444D+02 0.31433274D+02-0.21578039D+00 0.64057986D-03
-0.70572420D-06 0.26509150D-09-0.15490139D+06-0.12803880D+03
19  B203             69.64000          -0.2025670E+03
 0.83994106D+01 0.47436338D-02-0.19552304D-05 0.36187749D-09-0.24907232D-13
-0.10357158D+06-0.15823207D+02 0.36608837D+01 0.20262076D-01-0.21947338D-04
 0.12253004D-07-0.27038402D-11-0.10236524D+06 0.80930146D+01
20  B303CL3        186.83099          -0.3960570E+03
 0.19282564D+02 0.63172581D-02-0.27242926D-05 0.52047910D-09-0.36677790D-13
-0.20320883D+06-0.67898332D+02 0.40444983D+01 0.54260597D-01-0.55750761D-04
 0.22223128D-07-0.14181295D-11-0.19941632D+06 0.90435427D+01
21  B303F3         137.46001          -0.5704840E+03
 0.16858616D+02 0.88585754D-02-0.37881058D-05 0.71870401D-09-0.50376917D-13
-0.29093104D+06-0.59871948D+02 0.30798861D+01 0.45636592D-01-0.33098826D-04
 0.25538839D-08 0.44358761D-11-0.28712213D+06 0.11462196D+02
22  C(S)            12.01100          -0.2520000E+00
 0.13604942D+01 0.19182237D-02-0.84040389D-06 0.16448707D-09-0.11672670D-13
-0.65713870D+03-0.80070207D+01-0.44778053D+00 0.53691002D-02-0.39775571D-06
-0.40459298D-08 0.21134939D-11-0.94280688D+02 0.16840791D+01
23  C               12.01100           0.1693240E+03
 0.25810663D+01-0.14696202D-03 0.74388084D-07-0.79481079D-11 0.58900977D-16
 0.85216294D+05 0.43128879D+01 0.25328705D+01-0.15887641D-03 0.30682082D-06
-0.26770064D-09 0.87488827D-13 0.85240422D+05 0.46062374D+01
24  CH              13.01912           0.1399140E+03
 0.22673116D+01 0.22043000D-02-0.62250191D-06 0.69689940D-10-0.21274952D-14
 0.70838037D+05 0.87889352D+01 0.35632752D+01-0.20031372D-03-0.40129814D-06
 0.18226922D-08-0.86768311D-12 0.70405506D+05 0.17628023D+01
25  CH2             14.02709           0.8997400E+02
 0.27525479D+01 0.39782047D-02-0.14921731D-05 0.25956899D-09-0.17110673D-13
 0.45547759D+05 0.66534799D+01 0.35883347D+01 0.21724137D-02-0.13323408D-05
 0.19469445D-08-0.89431394D-12 0.45315188D+05 0.22627869D+01
26  CH20            30.02700          -0.3009400E+02
 0.28364249D+01 0.68605298D-02-0.26882647D-05 0.47971258D-09-0.32118406D-13
-0.15236031D+05 0.78531169D+01 0.37963783D+01-0.25701785D-02 0.18548815D-04
-0.17869177D-07 0.55504451D-11-0.15088947D+05 0.47548163D+01
27  CH3             15.03506           0.3233300E+02
 0.28400327D+01 0.60869086D-02-0.21740338D-05 0.36042576D-09-0.22725300D-13
 0.16449813D+05 0.55056751D+01 0.34666350D+01 0.38301845D-02 0.10116802D-05
-0.18859236D-08 0.66803182D-12 0.16313104D+05 0.24172192D+01
28  CH4             16.04300          -0.2029100E+02
 0.15027072D+01 0.10416798D-01-0.39181522D-05 0.67777899D-09-0.44283706D-13
-0.99787078D+04 0.10707143D+02 0.38261932D+01-0.39794581D-02 0.24558340D-04
-0.22732926D-07 0.69626957D-11-0.10144950D+05 0.86690073D+00
29  CO              28.01055          -0.2848900E+02
 0.29840696D+01 0.14891390D-02-0.57899684D-06 0.10364577D-09-0.69353550D-14
-0.14245228D+05 0.63479156D+01 0.37100928D+01-0.16190964D-02 0.36923594D-05
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-0.20319674D-08 0.23953344D-12-0.14356310D+05 0.29555351D+01
30  CO2                44.00995          -0.9629200E+02
 0.44608041D+01 0.30981719D-02-0.12392751D-05 0.22741325D-09-0.15525954D-13
-0.48961442D+05-0.98635982D+00 0.24007797D+01 0.87350957D-02-0.66070878D-05
 0.20021861D-08 0.63274039D-15-0.48377527D+05 0.96951457D+01
31  COCL               63.46355          -0.1776100E+02
 0.54291236D+01 0.16121535D-02-0.66006280D-06 0.12127114D-09-0.82858601D-14
-0.93305007D+04 0.36971816D+00 0.42863792D+01 0.50868980D-02-0.50729411D-05
 0.29647983D-08-0.77093453D-12-0.90125212D+04 0.62380308D+01
32  COCL2              98.92500          -0.5567500E+02
 0.77318082D+01 0.24089287D-02-0.10111133D-05 0.18936214D-09-0.13139356D-13
-0.29136566D+05-0.11221674D+02 0.31156139D+01 0.18478674D-01-0.22420544D-04
 0.12868184D-07-0.27360805D-11-0.28043884D+05 0.11755299D+02
33  C2H2               26.03800          0.5179700E+02
 0.45751083D+01 0.51238358D-02-0.17452354D-05 0.28673065D-09-0.17951426D-13
 0.25607428D+05-0.35737940D+01 0.14102768D+01 0.19057275D-01-0.24501390D-04
 0.16390872D-07-0.41345447D-11 0.26188208D+05 0.11393827D+02
34  C2H4               28.05418          0.1002600E+02
 0.34552152D+01 0.11491803D-01-0.43651750D-05 0.76155095D-09-0.50123200D-13
 0.44773119D+04 0.26987959D+01 0.14256821D+01 0.11383140D-01 0.79890006D-05
-0.16253679D-07 0.67491256D-11 0.53370755D+04 0.14621819D+02
35  CL                 35.45700          0.2742300E+02
 0.29537796D+01-0.40792712D-03 0.15288342D-06-0.26384345D-10 0.17206581D-14
 0.13695677D+05 0.30667325D+01 0.20774281D+01 0.29487169D-02-0.43919732D-05
 0.24499776D-08-0.41007685D-12 0.13871928D+05 0.73136343D+01
36  CL-                35.45355          -0.5590000E+02
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-0.28874558D+05 0.41872868D+01 0.25000000D+01 0.00000000D+00 0.00000000D+00
 0.00000000D+00 0.00000000D+00-0.28874558D+05 0.41872871D+01
37  CLF                54.45140          -0.1426900E+02
 0.41550345D+01 0.43195995D-03-0.16153995D-06 0.30453169D-10-0.21170113D-14
-0.74382198D+04 0.22303899D+01 0.28480871D+01 0.47719011D-02-0.52877698D-05
 0.23634468D-08-0.24187423D-12-0.71277966D+04 0.87639116D+01
38  CLF3               92.44820          -0.4123200E+02
 0.89535967D+01 0.11722163D-02-0.50896188D-06 0.97563489D-10-0.68858731D-14
-0.22075968D+05-0.18094713D+02 0.28949119D+01 0.24718550D-01-0.35139323D-04
 0.22559591D-07-0.53261978D-11-0.20798640D+05 0.11368534D+02
39  CL2                70.90600          -0.2194000E+01
 0.43077814D+01 0.31182816D-03-0.15310807D-06 0.44511913D-10-0.43057753D-14
-0.13458251D+04 0.20566684D+01 0.31316886D+01 0.48997877D-02-0.69414463D-05
 0.44785641D-08-0.10621859D-11-0.10979696D+04 0.77833424D+01
40  CL2O               86.90540          0.1820500E+02
 0.64340062D+01 0.62728809D-03-0.26933252D-06 0.51076394D-10-0.35691545D-14
 0.84860530D+04-0.49498767D+01 0.32545238D+01 0.12799449D-01-0.17882460D-04
 0.11264383D-07-0.25964252D-11 0.91657423D+04 0.10558058D+02
41  E                  0.00055           0.0000000E+00
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-0.74537496D+03-0.11734026D+02 0.25000000D+01 0.00000000D+00 0.00000000D+00
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42  F                 18.99840          0.1730200E+02
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 0.87163617D+04 0.38067182D+01 0.28128740D+01-0.33023098D-05-0.12897310D-05
 0.16837365D-08-0.64587833D-12 0.86604019D+04 0.30984198D+01
43  F-              18.99895          -0.6220000E+02
 0.25000000D+01 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00
-0.31483638D+05 0.32516223D+01 0.25000000D+01 0.00000000D+00 0.00000000D+00
 0.00000000D+00 0.00000000D+00-0.31483638D+05 0.32516223D+01
44  FO              34.99800          0.2390500E+02
 0.39192774D+01 0.70442345D-03-0.26648204D-06 0.49617599D-10-0.33688571D-14
 0.11798193D+05 0.33155951D+01 0.29680024D+01 0.26483393D-02-0.37368005D-06
-0.19006225D-08 0.10614283D-11 0.12087844D+05 0.83803342D+01
45  FO2             50.99720          0.3120000E+00
 0.57040935D+01 0.13862889D-02-0.58355374D-06 0.10937214D-09-0.75869181D-14
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 0.17562504D-08 0.67757430D-13 0.12769468D+03 0.78225198D+01
46  F2              38.00000          -0.2110000E+01
 0.40397806D+01 0.60869035D-03-0.21494672D-06 0.40596803D-10-0.28294433D-14
-0.13123536D+04 0.99528039D+00 0.28445997D+01 0.40135072D-02-0.32165655D-05
 0.47418780D-09 0.35556237D-12-0.99911761D+03 0.71131622D+01
47  F2O             53.99620          0.3256000E+01
 0.60051871D+01 0.11028402D-02-0.47547937D-06 0.90683145D-10-0.63757098D-14
 0.91906065D+03-0.52352686D+01 0.26109219D+01 0.12231280D-01-0.13441415D-04
 0.58909412D-08-0.57487175D-12 0.17347196D+04 0.11774719D+02
48  H               1.00797           0.5061900E+02
 0.25000000D+01 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00
 0.25471627D+05-0.46011763D+00 0.25000000D+01 0.00000000D+00 0.00000000D+00
 0.00000000D+00 0.00000000D+00 0.25471627D+05-0.46011762D+00
49  H2              2.01600           -0.2024000E+01
 0.31001901D+01 0.51119464D-03 0.52644210D-07-0.34909973D-10 0.36945345D-14
-0.87738042D+03-0.19629421D+01 0.30574451D+01 0.26765200D-02-0.58099162D-05
 0.55210391D-08-0.18122739D-11-0.98890474D+03-0.22997056D+01
50  H2O             18.01600          -0.6016500E+02
 0.27167633D+01 0.29451374D-02-0.80224374D-06 0.10226682D-09-0.48472145D-14
-0.29995826D+05 0.66305671D+01 0.40701275D+01-0.11084499D-02 0.41521180D-05
-0.29637404D-08 0.80702103D-12-0.30279722D+05-0.32270046D+00
51  HBO             27.82800          -0.2221500E+02
 0.39902785D+01 0.35116761D-02-0.41677746D-05 0.25804765D-09-0.17539792D-13
-0.11539403D+05 0.41315742D+00 0.27006640D+01 0.67921406D-02-0.48161185D-05
 0.21375092D-08-0.48790703D-12-0.11132099D+05 0.72359559D+01
52  HBO2            43.82800          -0.1365540E+03
 0.47389519D+01 0.47718771D-02-0.18063494D-05 0.31492889D-09-0.20738312D-13
-0.69248838D+05-0.33346713D-02 0.28707866D+01 0.78862644D-02-0.40736842D-06
-0.47059022D-08 0.23548893D-11-0.68624111D+05 0.10167320D+02
53  H3B3O6          131.48399         -0.5484400E+03
 0.20153579D+02 0.13016286D-01-0.50669619D-05 0.90308253D-09-0.60532410D-13
-0.28104092D+06-0.79689531D+02-0.22705116D+01 0.87024894D-01-0.91587714D-04
 0.39445392D-07-0.36666035D-11-0.27569523D+06 0.32516454D+02
54  HCL             36.46500          -0.2412800E+02
 0.27665884D+01 0.14381883D-02-0.46993000D-06 0.73499408D-10-0.43731106D-14
-0.11917468D+05 0.64583540D+01 0.35248171D+01 0.29984862D-04-0.86221891D-06
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 0.20979721D-08-0.98658191D-12-0.12150509D+05 0.23957713D+01
55  CHO            29.01900          -0.52870000E+01
 0.34738348D+01 0.34370227D-02-0.13632664D-05 0.24928645D-09-0.17044331D-13
 0.39594005D+04 0.60453340D+01 0.38840192D+01-0.82974448D-03 0.77900809D-05
-0.70616962D-08 0.19971730D-11 0.40563860D+04 0.48354133D+01
56  HF             20.00637          -0.67195000E+02
 0.30019188D+01 0.69528935D-03-0.56135180D-07-0.14767711D-10 0.22140435D-14
-0.33624997D+05 0.37575868D+01 0.34659720D+01 0.33246861D-03-0.10063786D-05
 0.12078301D-08-0.37137269D-12-0.33821824D+05 0.10758272D+01
57  HNO            31.01600          0.2141300E+02
 0.35548619D+01 0.32713182D-02-0.12734071D-05 0.22602046D-09-0.15064827D-13
 0.10693734D+05 0.51684901D+01 0.37412008D+01-0.20067061D-03 0.75409300D-05
-0.79105713D-08 0.25928389D-11 0.10817845D+05 0.50063473D+01
58  HO2            33.00800          0.2610000E+01
 0.37866280D+01 0.27885404D-02-0.10168708D-05 0.17183946D-09-0.11021852D-13
 0.11888500D+04 0.48147611D+01 0.35094850D+01 0.11499670D-02 0.58784259D-05
-0.77795519D-08 0.29607883D-11 0.13803331D+04 0.68276325D+01
59  H2O2           34.01600         -0.3512400E+02
 0.45731667D+01 0.43361363D-02-0.14746888D-05 0.23489037D-09-0.14316536D-13
-0.18006961D+05 0.50113696D+00 0.33887536D+01 0.65692260D-02-0.14850126D-06
-0.46258055D-08 0.24715147D-11-0.17663147D+05 0.67853631D+01
60  K+             39.10000          0.1228960E+03
 0.25000000D+01 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00
 0.61096558D+05 0.43339455D+01 0.25000000D+01 0.00000000D+00 0.00000000D+00
 0.00000000D+00 0.00000000D+00 0.61096558D+05 0.43339455D+01
61  K              39.10000          0.1982900E+02
 0.25673650D+01-0.14933596D-03 0.12342444D-06-0.53394240D-10 0.11948426D-13
 0.99550531D+04 0.46642081D+01 0.24930967D+01 0.50164177D-04-0.12751224D-06
 0.13540491D-09-0.51145936D-13 0.99786360D+04 0.50560438D+01
62  KCL            74.55500          -0.5367200E+02
 0.44636733D+01 0.12229207D-03-0.91719210D-08 0.92648242D-12-0.10407917D-16
-0.27173133D+05 0.32349330D+01 0.39908569D+01 0.21089169D-02-0.31836530D-05
 0.22525308D-08-0.59094179D-12-0.27080184D+05 0.54988475D+01
63  KO             55.10140          0.1469000E+02
 0.44244778D+01 0.19936155D-03-0.37128837D-07 0.71308300D-11-0.50369687D-15
 0.72052331D+04 0.32945055D+01 0.37470778D+01 0.31242017D-02-0.48020039D-05
 0.34660605D-08-0.93599791D-12 0.73368714D+04 0.65537609D+01
64  KOH            56.10937          -0.5800000E+02
 0.56400949D+01 0.12510226D-02-0.34984547D-06 0.44566993D-10-0.20870279D-14
-0.29698732D+05-0.40568187D+01 0.40733441D+01 0.97217945D-02-0.15988804D-04
 0.12143435D-07-0.33709342D-11-0.29506558D+05 0.29222373D+01
65  N              14.00800          0.1114484E+03
 0.24502682D+01 0.10661458D-03-0.74653373D-07 0.18796524D-10-0.10259839D-14
 0.56116040D+05 0.44487581D+01 0.25030714D+01-0.21800181D-04 0.54205287D-07
-0.56475602D-10 0.20999044D-13 0.56098904D+05 0.41675764D+01
66  N2             28.01340          -0.2072000E+01
 0.28963194D+01 0.15154866D-02-0.57235277D-06 0.99807393D-10-0.65223555D-14
-0.90586184D+03 0.61615148D+01 0.36748261D+01-0.12081500D-02 0.23240102D-05
-0.63217559D-09-0.22577253D-12-0.10611588D+04 0.23580424D+01
67  NA+            22.99100          0.1457550E+03
```

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 0.25000000D+01 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00
 0.72599329D+05 0.35374014D+01 0.25000000D+01 0.00000000D+00 0.00000000D+00
 0.0000000D+00 0.0000000D+00 0.72599330D+05 0.35374014D+01
68  NA              22.99100          0.2427400E+02
 0.25623078D+01-0.13963284D-03 0.11292708D-06-0.42307732D-10 0.67057055D-14
 0.12193782D+05 0.38957727D+01 0.24881226D+01 0.85426102D-04-0.21514228D-06
 0.22671887D-09-0.85125266D-13 0.12215904D+05 0.42804839D+01
69  NACL            58.44800         -0.4565800E+02
 0.44282931D+01 0.15527241D-03-0.28108383D-07 0.47163571D-11-0.28832557D-15
-0.23170900D+05 0.22878194D+01 0.37032286D+01 0.31997608D-02-0.48924502D-05
 0.34639218D-08-0.91357521D-12-0.23028276D+05 0.5760324 3D+01
70  NAO             38.98920          0.1774700E+02
 0.43924158D+01 0.21320574D-03-0.45220598D-07 0.79751821D-11-0.51735989D-15
 0.87118995D+04 0.23749268D+01 0.34421007D+01 0.41617241D-02-0.63118368D-05
 0.44479199D-08-0.11720486D-11 0.89011447D+04 0.69371625D+01
71  NAOH            39.99717         -0.5295000E+02
 0.56469377D+01 0.12227385D-02-0.33271036D-06 0.40666298D-10-0.17790688D-14
-0.25508222D+05-0.50500390D+01 0.40050388D+01 0.99922043D-02-0.16434213D-04
 0.12476585D-07-0.34637610D-11-0.25300471D+05 0.22932717D+01
72  NF              33.00510          0.5741000E+02
 0.38624046D+01 0.74409951D-03-0.29304178D-06 0.55130022D-10-0.38317928D-14
 0.28669390D+05 0.34570237D+01 0.30480682D+01 0.19566867D-02 0.94322448D-06
-0.29336643D-08 0.13504454D-11 0.28941688D+05 0.79092363D+01
73  NF2             52.00800          0.7572000E+01
 0.57186890D+01 0.14102822D-02-0.60493969D-06 0.11491911D-09-0.80536431D-14
 0.30992968D+04-0.34469259D+01 0.25009872D+01 0.10721062D-01-0.92064150D-05
 0.19027666D-08 0.71249647D-12 0.39376954D+04 0.12994042D+02
74  NF3             71.00190         -0.3426200E+02
 0.79819180D+01 0.22349897D-02-0.96301027D-06 0.18357806D-09-0.12901442D-13
-0.18673358D+05-0.15667394D+02 0.12676904D+01 0.24289231D-01-0.26835971D-04
 0.11994191D-07-0.12905657D-11-0.17059051D+05 0.17977633D+02
75  NH              15.01467          0.7894000E+02
 0.27789900D+01 0.13266349D-02-0.41101218D-06 0.69414505D-10-0.44536190D-14
 0.44567973D+05 0.57593434D+01 0.34938318D+01 0.24529034D-03-0.12578521D-05
 0.22011922D-08-0.92288834D-12 0.44326826D+05 0.18451723D+01
76  NH2             16.02254          0.3769700E+02
 0.25769524D+01 0.35896090D-02-0.12276328D-05 0.19549576D-09-0.11873401D-13
 0.19335912D+05 0.79074890D+01 0.40385791D+01-0.10098163D-02 0.40120903D-05
-0.23085312D-08 0.39022887D-12 0.18973010D+05 0.52464285D+00
77  NH3             17.03061         -0.1337400E+02
 0.24165177D+01 0.61871211D-02-0.21785136D-05 0.37599090D-09-0.24448856D-13
-0.64747177D+04 0.77043482D+01 0.35912769D+01 0.49388668D-03 0.83449322D-05
-0.83833385D-08 0.27299092D-11-0.66717143D+04 0.22520966D+01
78  ND+             30.00555          0.2366600E+03
 0.28885488D+01 0.15217119D-02-0.57531241D-06 0.10051081D-09-0.66044294D-14
 0.11819245D+06 0.70027197D+01 0.36685056D+01-0.11544580D-02 0.21755608D-05
-0.48227472D-09-0.27847906D-12 0.11803369D+06 0.31779324D+01
79  ND              30.00800         -2.1970000E+00
 0.31890000D+01 0.13382281D-02-0.52899318D-06 0.95919332D-10-0.64847932D-14
 0.98283290D+04 0.67458126D+01 0.40459521D+01-0.34181783D-02 0.79819190D-05
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-0.611393160-08 0.15919076D-11 0.97453934D+04 0.29974988D+01
80  NOCL                65.45910        0.9657000E+01
 0.54178186D+01 0.17391415D-02-0.67354352D-06 0.12747721D-09-0.88128378D-14
 0.44207903D+04-0.15287316D+00 0.40453848D+01 0.58322333D-02-0.54789276D-05
 0.27968775D-08-0.59348675D-12 0.47980577D+04 0.68935321D+01
81  NOF                 49.01000       -0.1825800E+02
 0.51906666D+01 0.18924266D-02-0.78642361D-06 0.14626364D-09-0.10097419D-13
-0.96758164D+04-0.62298477D+00 0.32902070D+01 0.74045493D-02-0.66195803D-05
 0.26529282D-08-0.29526815D-12-0.91566645D+04 0.91451185D+01
82  NO2                 46.00800       -2.4350000E+00
 0.46240771D+01 0.25260332D-02-0.10609498D-05 0.19879239D-09-0.13799384D-13
 0.22899900D+04 0.13324138D+01 0.34589236D+01 0.20647064D-02 0.66866067D-05
-0.95556725D-08 0.36195881D-11 0.28152265D+04 0.83116983D+01
83  N2O                 44.01600        0.1732000E+02
 0.47306679D+01 0.28258267D-02-0.11558115D-05 0.21263683D-09-0.14564087D-13
 0.81617682D+04-0.17151073D+01 0.26189196D+01 0.86439616D-02-0.68110624D-05
 0.22275877D-08-0.80650330D-13 0.87590123D+04 0.92266952D+01
84  N2O4                92.01600       -0.1749000E+01
 0.10506637D+02 0.58723267D-02-0.24766296D-05 0.46556024D-09-0.32402082D-13
-0.28609096D+04-0.26252230D+02 0.36662865D+01 0.23491748D-01-0.16007297D-04
 0.11845939D-08 0.20000161BD-11-0.90631797D+03 0.93973337D+01
85  O                   16.00000        0.5795100E+02
 0.25420596D+01-0.27550619D-04-0.31028033D-08 0.45510674D-11-0.43680515D-15
 0.29230803D+05 0.49203080D+01 0.29464287D+01-0.16381665D-02 0.24210316D-05
-0.16028432D-08 0.38906964D-12 0.29147644D+05 0.29639949D+01
86  O-                  15.99995        0.2430000E+02
 0.25437173D+01-0.53258700D-04 0.25119617D-07-0.51851466D-11 0.39011542D-15
 0.11480516D+05 0.45225238D+01 0.28115796D+01-0.11905697D-02 0.18710553D-05
-0.13479178D-08 0.36663554D-12 0.11428431D+05 0.32402855D+01
87  OH                  17.00740        0.7240000E+01
 0.29131230D+01 0.95418248D-03-0.19084325D-06 0.12730795D-10 0.24803941D-15
 0.39647060D+04 0.54288735D+01 0.38365518D+01-0.10702014D-02 0.94849757D-06
 0.20843575D-09-0.23384265D-12 0.36715807D+04 0.49805456D+00
88  OH-                 17.00790       -0.3440000E+02
 0.28881148D+01 0.96560229D-03-0.19659254D-06 0.14053802D-10 0.12080617D-15
-0.18086455D+05 0.41896259D+01 0.34621427D+01 0.40525802D-03-0.13516992D-05
 0.17899459D-08-0.63434810D-12-0.18312355D+05 0.92893220D+00
89  O2                  31.99880       -0.2075000E+01
 0.36219535D+01 0.73618264D-03-0.19652228D-06 0.36201558D-10-0.28945627D-14
-0.12019825D+04 0.36150960D+01 0.36255985D+01-0.18782184D-02 0.70554544D-05
-0.67635137D-08 0.21555993D-11-0.10475226D+04 0.43052778D+01
90  O2-                 31.99935       -0.1139000E+02
 0.38147234D+01 0.77444546D-03-0.30677649D-06 0.56618118D-10-0.38229492D-14
-0.69910087D+04 0.29587995D+01 0.31440525D+01 0.12127972D-02 0.23812161D-05
-0.40914092D-08 0.16885304D-11-0.67369752D+04 0.67688687D+01
91  AR                  39.948         -0.1481300E+01
-0.25000000D+01 0.00000000D+01 0.00000000D+01 0.00000000D+01 0.00000000D+01
-0.74537502D+03 0.43660006D+01 0.25000000D+01 0.00000000D+01 0.00000000D+01
 0.00000000D+01 0.00000000D+01-0.74537498D+03 0.43660006D+01
92  HE                  4.0026         -0.1481300E+01
```

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 0.25000000D+01 0.00000000D+01 0.00000000D+01 0.00000000D+01 0.00000000D+01
-0.74537498D+03 0.91534888D+00 0.25000000D+01 0.00000000D+01 0.00000000D+01
 0.00000000D+01 0.00000000D+01-0.74537498D+03 0.91534884D+00
93  O3            48.0          -0.2474000E+01
 0.55057580D+01 0.17201400D-02-0.72377700D-06 0.14005700D-09-0.99663500D-14
 0.15242580D+05-0.37193300D+01 0.22456605D+01 0.01077244D+00-0.90187700D-05
 0.22411200D-08 0.37815800D-12 0.16136905D+05 0.13097300D+02
94  H3O+          19.02345
2.5627          .0054530        -.0000017270   2.579400000D-10-1.48150000D-14
68948.245       7.0210          4.1556         -.0042686       .000021425
-2.38800000D-08 9.16160000D-12 68703.0         -.055377
95  H+            1.00745
 0.25000000D+01 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00
 0.18402490D+06-0.11591800D+01 0.25000000D+01 0.00000000D+00 0.00000000D+00
 0.00000000D+00 0.00000000D+00 0.18402490D+06-0.11691800D+01
96 OH+           17.00745
2.70906         .00151549       -.502280000D-06 .815266000E-10-.479012000D-14
157626.5        6.29659         3.44208         .000672536      -.255586000D-05
.394765000D-08-.171481000D-11   157375.0        2.24161
97  H2O+          18.01545
3.28744         .00212755       -.359547000D-06 .258697000D-10-.743394000D-15
117011.4        4.188           4.093981       -.166835000D-02 .684864000D-05
-.652035100D-08 .234055000D-11   116868.4        0.4051
98  NNH           29.024
 0.35548619D+01 0.32713182D-02-0.12734071D-05 0.22602046D-09-0.15064827D-13
 0.27400700D+05 0.51684901D+01 0.37412008D+01-0.20067061D-03 0.75409300D-05
-0.79105713D-08 0.25928389D-11 0.27524800D+05 0.50063473D+01
99  EXC1          18.01600        -0.6016500E+02
 0.27167633D+01 0.29451374D-02-0.80224374D-06 0.10226682D-09-0.48472145D-14
-0.29905826D+05 0.66305671D+01 0.40701275D+01-0.11084499D-02 0.41521180D-05
-0.29637404D-08 0.80702103D-12-0.30279722D+05-0.32270046D+00
100 EXC2          18.01600        -0.6016500E+02
 0.27167633D+01 0.29451374D-02-0.80224374D-06 0.10226682D-09-0.48472145D-14
-0.29905826D+05 0.66305671D+01 0.40701275D+01-0.11084499D-02 0.41521180D-05
-0.29637404D-08 0.80702103D-12-0.30279722D+05-0.32270046D+00
101 EXC3          18.01600        -0.6016500E+02
 0.27167633D+01 0.29451374D-02-0.80224374D-06 0.10226682D-09-0.48472145D-14
-0.29905826D+05 0.66305671D+01 0.40701275D+01-0.11084499D-02 0.41521180D-05
-0.29637404D-08 0.80702103D-12-0.30279722D+05-0.32270046D+00
102 ION2          37.0395
2.5627          .0054530        -.0000017270   2.579400000D-10-1.48150000D-14
68948.245       7.0210          4.1556         -.0042686       .000021425
-2.38800000D-08 9.16160000D-12 68703.0         -.055377
103 ION3          55.0555
2.5627          .0054530        -.0000017270   2.579400000D-10-1.48150000D-14
68948.245       7.0210          4.1556         -.0042686       .000021425
-2.38800000D-08 9.16160000D-12 68703.0         -.055377
104 ION4          73.0715
2.5627          .0054530        -.0000017270   2.579400000D-10-1.48150000D-14
68948.245       7.0210          4.1556         -.0042686       .000021425
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```
 -2.38800000D-08 9.16160000D-12 68703.0          -.055377
105  DBL          36.0320000          -1.2033000E+02
  0.27167633D+01 0.29451374D-02-0.80224374D-06 0.10226682D-09-0.48472145D-14
 -0.29905826D+05 0.66305671D+01 0.40701275D+01-0.11084499D-02 0.41521180D-05
 -0.29637404D-08 0.80702103D-12-0.30279722D+05-0.32270046D+00
106  OH           15.99945
  0.25000000D+01 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00
  0.18868400D+06 4.38100000D+00 0.25000000D+01 0.00000000D+00 0.00000000D+00
  0.00000000D+00 0.00000000D+00 0.18868400D+06 4.38100000D+00
107  S1           9.00800          -0.6016500E+02
  0.27167633D+01 0.29451374D-02-0.80224374D-06 0.10226682D-09-0.48472145D-14
 -0.29905826D+05 0.66305671D+01 0.40701275D+01-0.11084499D-02 0.41521180D-05
 -0.29637404D-08 0.80702103D-12-0.30279722D+05-0.32270046D+00
108  S2           18.02000          -0.6016500E+02
  0.27167633D+01 0.29451374D-02-0.80224374D-06 0.10226682D-09-0.48472145D-14
 -0.29905826D+05 0.66305671D+01 0.40701275D+01-0.11084499D-02 0.41521180D-05
 -0.29637404D-08 0.80702103D-12-0.30279722D+05-0.32270046D+00
END OF SPECIES CURVE FIT COEFFICIENTS
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          ZZ.CHEM+
COMMENT:  ADDED TO. TO INCLUDE SINGLE CARBON C-H REACTIONS COMPILE
BY PAMIDIMUKKALA AND GREEN
-----------------------------
   1 OH     +O                =H      +O2                18 3.0E-11 0.0-960.     +-0.2
   2 OH     +H                =H2     +O                 18 1.4E-14-1.0-7000.    +.2,-.1
   3 OH     +OH               =H2O    +O                 15 1.0E-11 0.0-1100.    +-0.5
   4 OH     +H2               =H2O    +H                 18 3.5E-11 0.0-5180.    +-0.3
   5 H      +H      +M        =H2     +M                 22 3.0E-30 1.0 0.       +-1.0
   6 H      +O      +M        =OH     +M                 22 1.0E-29 1.0 0.       +-1.5
   7 O      +O      +M        =O2     +M                 25 3.0E-34 0.0 1800.    +-0.5
   8 H      +OH     +M        =H2O    +M                 23 1.0E-25 2.0 0.       +-0.5
   9 OH     +CO               =CO2    +H                 18 2.8E-17-1.3 660.     +-0.3
  10 CO     +O      +M        =CO2    +M                 25 6.5E-33 0.0-4360.    +-1.0
  11 CL     +H2               =HCL    +H                 15 1.4E-11 0.0-4260.    +.7,-.5
  12 CL     +H2O              =HCL    +OH                15 5.0E-11 0.0-17600.   +-0.5
  13 HCL    +O                =OH     +CL                15 6.0E-12 0.0-6000.    +-1.0
  14 H      +CL2              =HCL    +CL                15 1.5E-10 0.0-1200.    +.3,-.5
  15 CL     +CL     +M        =CL2    +M                 25 1.0E-33 0.0 1800.    +-0.6
  16 H      +CL     +M        =HCL    +M                 23 4.0E-26 2.0 0.       +-1.0
  17 F      +H2               =HF     +H                 15 1.5E-10 0.0-1600.    +.3,-.7
  18 F      +H2O              =HF     +OH                15 2.2E-11 0.0-400.     +-1.0
  19 HF     +O                =OH     +F                 15 7.0E-11 0.0-33800.   +.6,-1.5
  20 H      +F2               =HF     +F                 15 2.0E-10 0.0-2400.    +.3,-1.0
  21 F      +F      +M        =F2     +M                 27 3.0E-30 1.5 0.       +-1.5
  22 H      +F      +M        =HF     +M                 22 2.5E-29 1.0 0.       +1.,-1.5
  23 BO     +O2               =BO2    +O                 11 3.0E-12 0.0 0.       +-2.0
  24 BO2    +H2               =HBO2   +H                 15 3.0E-12 0.0-3000.    +-2.0
  25 BO     +OH               =BO2    +H                 11 4.0E-12 0.0 0.       +-2.0
  26 BO2    +OH               =HBO2   +O                 15 3.0E-12 0.0-1000.    +-2.0
  27 BO     +H2O              =HBO2   +H                 15 1.0E-13 0.0-10000.   +-2.0
```

28	BO2	+H2O		=HBO2	+OH		15	2.0E-12	0.0-2460.	+-2.0
29	BO2	+BO2		=B2O3	+O		15	1.0E-13	0.0-10000.	+-2.0
30	B2O3	+H2O		=HBO2	+HBO2		15	1.0E-15	0.0-13000.	+-2.0
31	BF	+O		=BO	+F		11	8.0E-11	0.0 0.	+1.5,-2.
32	BF	+OH		=BOF	+H		11	2.0E-11	0.0 0.	+-2.0
33	BF	+O2		=BOF	+O		15	2.0E-11	0.0-5000.	+-2.0
34	BF2	+H		=BF	+HF		11	5.0E-11	0.0 0.	+-2.0
35	BF2	+O		=BOF	+F		11	2.0E-10	0.0 0.	+.3,-2.
36	BF2	+BO2		=BOF	+BOF		11	1.0E-12	0.0 0.	+-2.0
37	BF2	+BO		=BOF	+BF		11	1.0E-11	0.0 0.	+-2.0
38	BF3	+H		=BF2	+HF		15	3.5E-10	0.0-21060.	+.3,-2.
39	BO	+HF		=BOF	+H		15	3.0E-12	0.0-7000.	+-2.0
40	BO	+HCL		=BOCL	+H		15	3.0E-12	0.0-7000.	+-2.0
41	BO2	+HF		=BOF	+OH		15	3.0E-12	0.0-10000.	+-2.0
42	BO2	+F		=BOF	+O		11	2.0E-10	0.0 0.	+.3,-2.
43	BO2	+HCL		=BOCL	+OH		15	1.0E-12	0.0-3000.	+-2.0
44	BOCL	+OH		=BO2	+HCL		15	3.0E-10	0.0-5000.	+.3,-2.
45	BOCL	+O		=BO2	+CL		11	2.0E-10	0.0 0.	+.3,-2.
46	H	+O2	+M	=HO2	+M		25	4.1E-33	0.0 1000.	+-0.5
47	HO2	+H		=OH	+OH		15	4.2E-10	0.0-1900.	+.3,-.7
48	HO2	+H		=H2	+O2		15	4.2E-11	0.0-700.	+-0.7
49	HO2	+H2		=H2O2	+H		15	1.2E-12	0.0-18800.	+-0.5
50	HO2	+HO2		=H2O2	+O2		11	3.3E-12	0.0 0.	+-2.0
51	OH	+OH	+M	=H2O2	+M		25	2.5E-33	0.0 5100.	+-0.5
52	H2O2	+OH		=H2O	+HO2		15	1.7E-11	0.0-1820.	+-0.5
53	N	+O2		=NO	+O		18	1.1E-14-1.0-7300.		+-0.2
54	O	+N2		=NO	+N		15	1.3E-10	0.0-76000.	+-0.5
55	N	+OH		=NO	+H		15	1.0E-10	0.0-850.	+-0.5
56	NO2	+H		=NO	+OH		15	5.8E-10	0.0-1470.	+-0.5
57	NO2	+O		=NO	+O2		15	1.7E-11	0.0-600.	+-0.5
58	NO	+NO		=N2O	+O		15	2.2E-12	0.0-64200.	+-0.5
59	N2O	+H		=N2	+OH		15	1.3E-10	0.0-15200.	+-0.3
60	HNO	+H		=H2	+NO		11	8.0E-12	0.0 0.	+-0.7
61	HNO	+OH		=H2O	+NO		11	6.0E-11	0.0 0.	+-0.5
62	NO	+O	+M	=NO2	+M		24	1.8E-31	0.5 0.	+-0.5
63	NO	+H	+M	=HNO	+M		25	5.0E-32	0.0 600.	+-0.5
64	NO2	+NO2		=NO	+NO	+O2	35	3.3E-12	0.0-26900.	+-0.3
65	NACL	+H		=NA	+HCL		15	3.0E-11	0.0-780.	+-1.0
66	KCL	+H		=K	+HCL		15	3.2E-11	0.0-1080.	+-1.0
67	NAOH	+H		=NA	+H2O		15	3.5E-12	0.0-2200.	+-1.0
68	KOH	+H		=K	+H2O		15	3.6E-12	0.0-2000.	+-1.0
69	NA+	+E	+M	=NA	+M		22	4.0E-24	1.0 0.	+-0.5
70	K+	+E	+M	=K	+M		22	4.0E-24	1.0 0.	+-0.5
71	NA+	+CL-		=NA	+CL		14	2.2E-08	0.5 0.	+.5,-1.
72	K+	+CL-		=K	+CL		14	1.7E-09	0.5 0.	+-1.0
73	NA+	+CL-	+M	=NACL	+M		28	5.5E-16	3.5-1500.	+-1.0
74	K+	+CL-	+M	=KCL	+M		28	1.6E-15	3.5-4800.	+-1.0
75	NA+	+OH-	+M	=NAOH	+M		24	1.0E-08	0.5 0.	+-2.0
76	K+	+OH-	+M	=KOH	+M		24	1.0E-08	0.5 0.	+-2.0
77	HCL	+E		=CL-	+H		15	1.4E-07	0.0-15200.	+.3,-3.

78	CL	+E	+M	=CL-	+M	
79	OH	+E	+M	=OH-	+M	
80	B	+O2		=BO	+O	
81	B	+OH		=BO	+H	
82	B	+BO2		=BO	+BO	
83	BO	+O	+M	=BO2	+M	
84	BO2	+H	+M	=HBO2	+M	
85	BO	+OH	+M	=HBO2	+M	
86	BO	+BO2	+M	=B2O3	+M	
87	B	+HF		=BF	+H	
88	B	+HCL		=BCL	+H	
89	BCL	+O2		=BOCL	+O	
90	BCL	+O		=BO	+CL	
91	BCL	+OH		=BOCL	+H	
92	BF2	+BF2		=BF3	+BF	
93	BFCL	+H		=HCL	+BF	
94	BFCL	+H		=HF	+BCL	
95	BFCL	+OH		=HF	+BOCL	
96	BFCL	+OH		=HCL	+BOF	
97	BFCL	+O		=BOF	+CL	
98	BFCL	+O		=BOCL	+F	
99	BFCL	+BF2		=BF3	+BCL	
100	BFCL	+BO		=BOF	+BCL	
101	BFCL	+BO		=BOCL	+BF	
102	BFCL	+BO2		=BOCL	+BOF	
103	BFCL	+BF		=BF2	+BCL	
104	BF2	+OH		=BOF	+HF	
105	NO	+O3		=NO2	+O2	
106	H2	+O2		=OH	+OH	
107	OH	+HO2		=H2O	+O2	
108	O	+HO2		=O2	+OH	
109	CH4	+OH		=CH3	+H2O	
110	CH4	+H		=CH3	+H2	
111	CH4	+O		=CH3	+OH	
112	CH4	+M		=CH3	+H	+M
113	CH3	+O		=CH2O	+H	
114	CH3	+O2		=CH2O	+OH	
115	CH3	+O2		=CHO	+H2O	
116	CH3	+OH		=CH2	+H2O	
117	CH3	+OH		=CH2O	+H2	
118	CH3	+O		=CHO	+H2	
119	CH3	+H		=CH2	+H2	
120	CH2O	+M		=CO	+H2	+M
121	CH2O	+M		=CHO	+H	+M
122	CH2O	+OH		=CHO	+H2O	
123	CH2O	+O		=CHO	+OH	
124	CH2O	+H		=CHO	+H2	
125	CHO	+M		=CO	+H	+M
126	CHO	+O2		=CO	+HO2	
127	CHO	+O2		=CO2	+OH	

25	1.0E-32	0.0	6000.	+-1.5
21	3.0E-31	0.0	0.	+1.,-2.
11	8.0E-11	0.0	0.	+1.5,-2.
11	6.0E-11	0.0	0.	+.3,-2.
11	6.0E-11	0.0	0.	+1.,-2.
25	3.0E-33	0.0	2000.	+-2.0
25	5.0E-33	0.0	2000.	+-2.0
25	1.0E-33	0.0	2000.	+-2.0
25	5.0E-35	0.0	2000.	+-2.5
11	6.0E-10	0.0	0.	+.1,-2.
11	6.0E-10	0.0	0.	+.1,-2.
15	2.0E-11	0.0-5000.		+1.3,-2.
11	5.0E-10	0.0	0.	+.1,-2.
15	2.0E-11	0.0-5000.		+-2.0
11	1.0E-12	0.0	0.	+-2.0
11	2.0E-10	0.0	0.	+.3,-2.
11	4.0E-11	0.0	0.	+1.,-2.
15	1.0E-12	0.0-10000.		+-2.0
15	2.0E-12	0.0-10000.		+-2.0
11	2.0E-10	0.0	0.	+.3,-2.
11	5.0E-11	0.0	0.	+.5,-2.
11	1.0E-12	0.0	0.	+-2.0
11	5.0E-12	0.0	0.	+-2.0
11	5.0E-12	0.0	0.	+-2.0
11	1.0E-12	0.0	0.	+-2.0
11	5.0E-12	0.0	0.	+1.5,-2.
15	3.0E-12	0.0-5000.		+-2.0
65	9.0E-13	0.0-2500.		
15	2.8E-11	0.0-47780.		
11	2.0E-11	0.0	0.	
11	1.7E-11	0.0	0.	
15	5.0E-11	0.0-5007.		+-.
15	3.3E-10	0.0-11902.		+-.3
15	3.3E-11	0.0-6895.		+-.
55	3.3E-07	0.0-88422.		
15	1.2E-10	0.0-994.		
15	5.0E-11	0.0-17506.		
11	3.3E-14	0.0	0.	
18	1.0E-13	-0.7-2007.		
11	6.6E-12	0.0	0.	
11	1.7E-10	0.0	0.	
18	2.6E-10	0.3-12439.		
55	3.3E-08	0.0-35011.		
55	6.6E-12	0.0-36760.		
15	4.2E-11	0.0-994.		
11	5.0E-11	0.0	0.	
15	2.8E-11	0.0-3000.		
58	3.3E-12	-0.5-28812.		
11	5.0E-11	0.0	0.	
18	1.2E-12	-0.5	0.	

```
128 CHO    +O                =CO     +OH                 18 8.9E-13-0.5 0.
129 CHO    +O                =CO2    +H                  18 8.9E-13-0.5 0.
130 CHO    +OH               =CO     +H2O                11 1.7E-10 0.0 0.
131 CHO    +H                =CO     +H2                 18 2.6E-12-0.5 0.
132 CO     +OH               =CO2    +H                  15 9.1E-13 0.0-1073.
133 CO     +O       +M       =CO2    +M                  26 6.0E-09 1.0-2504.
134 CO     +O2               =CO2    +O                  15 2.6E-11 0.0-40992.
135 H      +O2               =OH     +O                  15 3.6E-10 0.0-16810.
136 CH2    +OH               =CH     +H2O                18 8.3E-13-0.5-5961.
137 CH2    +O                =CH     +OH                 18 3.3E-13-0.7-25831.
138 CH2    +O                =CHO    +H                  18 8.3E-13-0.5-4000.
139 CH2    +O2               =CH2O   +O                  18 8.3E-13-0.5-7000.
140 CH2    +H                =CH     +H2                 18 5.3E-13-0.7-5000.
141 CH     +O2               =CHO    +O                  18 8.3E-13-0.5-6000.
142 CH     +OH               =CHO    +H                  18 8.3E-13-0.5-10000.
143 CH     +O                =CO     +H                  14 1.0E-12-0.5 0.0
144 CH     +HO2              =CH2    +O2                 18 2.0E-14-0.5-15100.
145 CH     +HO2              =CHO    +OH                 18 8.3E-13-0.5-6000.
146 CH     +CHO              =CH2    +CO                 18 5.3E-13-0.7-1000.
-----------------------------
          MKREACT
COMMENT: H-O REACTIONS LISTED IN MILLER AND KEE (1978).  SEE BIBLIOG.
-----------------------------
147 H2     +O2               =OH     +OH                 15 2.8E-11 0.0-47780.
148 H2     +OH               =H2O    +H                  15 8.6E-11 0.0-6500.
149 H      +O2               =OH     +O                  18 2.0E-07 .91-16620.
150 O      +H2               =OH     +H                  18 3.0E-14 -1.-8826.
151 H      +O2      +M       =HO2    +M                  25 5.5E-33 0.0 870.
152 OH     +HO2              =H2O    +O2                 11 2.0E-11 0.0 0.
153 H      +HO2              =OH     +OH                 11 1.0E-10 0.0 0.
154 O      +HO2              =O2     +OH                 11 1.7E-11 0.0 0.
155 OH     +OH               =O      +H2O                18 2.8E-18 -2. 1190.
156 H2     +M                =H      +H       +M         58 3.7E-12 -.5 -92600.
157 H2     +H2O              =H      +H       +H2O       38 1.5E-11 -.5 -92600.
158 O2     +M                =O      +O       +M         58 3.1E-13 -.5 -95560.
159 H      +OH      +M       =H2O    +M                  28 2.1E-24 2.6 0.
160 H2O    +H2O              =H      +OH      +H2O       35 6.8E-07 0.0-105000.
161 O      +N2               =NO     +N                  15 2.3E-10 0.0 -75800.
162 N      +O2               =NO     +O                  18 1.1E-14 -1. -6280.
163 OH     +N                =NO     +H                  11 6.6E-11 0.0 0.
164 H      +HO2              =H2     +O2                 11 2.2E-11 0.0 0.
-----------------------------
          COMP81FB
COMMENT:  H-O REACTIONS FROM COMPILATION OF WESTBROOK (1981).  SEE BIBLIOG.
-----------------------------
INCLUDE COMP81FB 20035006,12
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          ADDDDD
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C
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C
C     THIS VERSION HAS  25 SPECIES; 80 CHEMICAL REACTIONS; 101 GRID PTS
C     NRX=80  NUMBER OF CHEMICAL REACTIONS
C     NSX=25  NUMBER OF SPECIES
C     MPSIX=101  NUMBER OF XI GRID PTS.  MAX NUMBER OF ETA GRID PTS = 61
C
C234567890123456789 123456789 123456789 123456789 123456789 123456789 1234567890
C 69
      DIMENSION Y(101), PSI(101), R(101), Z(101), RHO(101)
      DIMENSION H1(101), H2(101), R1(101), R2(101), Z1(101), Z2(101)
      DIMENSION ALPHA(25,101), RALPHA(25,101),    ETA(61)
      DIMENSION AID(25), WTMOLE(25), G(25), WP(25), WM(25), QX(25)
      DIMENSION CM(25,25),     A(101), TRIP(101),     YI(25,101)
      DIMENSION RC(80,3), IRRR(80,5), IRR(80), IRT(80), ZID(5)
      DIMENSION CON(14,25), J12345(5), TITLE(18)
      DIMENSION AL(25), BL(25), CL(25), DFCOEF(25),    ZZ0(101)
      DIMENSION R1P(101), Z1P(101), H1P(101), DPDY(101), DINVD(101)
      DIMENSION       ALF(25,101)
      DIMENSION XCHANG(20), PRNTXC(20),  BETA(25,101)
C
      DIMENSION BB(101), ATA(101), PXI0(8), PXX1(8)
      DIMENSION PXX2(3), PXX3(8)
C
      DIMENSION RPRM(8900)
C
      EQUIVALENCE (J1, J12345(1))
      EQUIVALENCE (ALPHA(1), BETA(1))
C
      COMMON    BB, BBO, XIB, PB,      XIO,  XCOR, DXINIT
      COMMON                      XIOIN,    B23D
C
      COMMON    ALPHA,  RALPHA,  WTMOLE,  AID,  TITLE,  G,  WTMIX
      COMMON    WM,  WP,  RC,  CON,  X,  XMAX,  PRNT,  DXMIN,  DX
      COMMON    FDL,  DFDL,  DELPSI,  ZID,  IRRR,  IRR,  IRT
      COMMON    IFINIS,  IPAGE,  MPSI,  NS,  NR,  NPSI,  LPSI
      COMMON    IOUT,  NT,  XINIT
      COMMON    PCNT,  XD,  XCHANG,  PRNTXC,  CM,  QX,  J1,J2,J3,J4,J5
      COMMON  TEMRP, TEMRM,   CRR,   ITFLG,  AL,BL,CL,   MPSIX, NSX, NRX
C  TEMRP, TEMRM MUST BE IN THIS ORDER. J1, J2, J3, J4, J5 MUST BE IN THIS
C  ORDER.
      COMMON    Y,  YR,  PSI,  RHO,  R,  H1,  H2,  R1,  R2,  Z1,  Z2
      COMMON    ETA, NET, IET, ETAT,  DFCOEF,    E0, T, DENS, RATEIN, Z0
      COMMON    ATA, XIEDGE
      COMMON    A, TRIP,  DFCOMX,  RO,       YI,       Z, ZZ0
      COMMON    R1P,  Z1P,    H1P,  DPDY,    DINVD
      COMMON     IXC, NXC,       ALF, IRS, IXX, IIN, IMF, IINT, NSTEP
      COMMON     IPR, CPR, CCHM, CINT, XIOINT, IDIAG, JH20, IREAC
      COMMON PXI0, PXX1, PXX2, PXX3
C
      COMMON RPRM
```

```
C
-----------------------------
            B.MODK
-----------------------------
C
      IDIAG = 0
C
      CALL ERRSET(208,2000,-1,1)
C  SUPPRESS UNDERFLOW ERROR MESSAGES
      CALL BOATSA
C
      CALL PREP( RO, RATEIN )
C  NOTE:  RO IS MASS DENSITY IN GM/CC.  DENS IS NUMBER DENSITY IN #/CC.
C
      DO 20 IET = 1, NET
      ETAT = ETA(IET)
      CALL BOATSB
   10 CALL BOATMI
      IF(ITFLG .LE. 0) GO TO 10
      CALL BOATOI
   20 CONTINUE
      WRITE(6,101)
  101 FORMAT(1H0,'END OF ETA GRID')
      STOP
      END
-----------------------------
            B.UT
-----------------------------
      SUBROUTINE BOATLI(XIN,YOUT,XXX,YYY,N)
C
      DIMENSION XXX(101),YYY(101)
      K=2
   20 IF(XIN.LE.XXX(K)) GO TO 10
      K=K+1
      IF(K.GT.N) WRITE(6,100)
      IF(K.GT.N) K=N
      IF(K.EQ.N) GO TO 10
      GO TO 20
   10 RAT=(XIN-XXX(K-1))/(XXX(K)-XXX(K-1))
      YOUT=YYY(K-1)+RAT*(YYY(K)-YYY(K-1))
      RETURN
  100 FORMAT(36H *****   K .GT. N  IN  BOATLI  *****)
      END
      SUBROUTINE BOATSL(X,A,N)
C     THIS PROGRAM FINDS THE SOLUTIONS TO A SET OF N SIMULTANEOUS LINEAR
C     EQUATIONS BY USING THE GAUSS-JORDAN REDUCTION ALGORITHM WITH THE
C     DIAGONAL PIVOT STRATEGY
      DIMENSION A(25,25),X(25)
      DO 9 K=1,N
      IF (ABS(A(K,K)) .GT. 1.E-10) GO TO 5
```

```
      WRITE(6,101)
      GO TO 99
    5 KP1= K+1
      DO 6 J= KP1, N
    6 A(K,J)= A(K,J)/A(K,K)
      X(K)= X(K)/A(K,K)
      A(K,K)= 1.0
      DO 9 I=1,N
      IF (I.EQ.K .OR. A(I,K).EQ.0.) GO TO 9
      DO 8 J=KP1,N
    8 A(I,J)= A(I,J)- A(I,K)*A(K,J)
      X(I)= X(I)- A(I,K)*X(K)
      A(I,K)=0.
    9 CONTINUE
  101 FORMAT( 22H ERROR--- SMALL PIVOT )
   99 RETURN
      END
C
C - - - - - - - - - - - - - -
C
      SUBROUTINE SFVFL (VAL, VEC, NW)
C
C     SFVFL - STANDARD FORTRAN VECTOR FILL
C
      DIMENSION VEC(1)
      DO 10 I = 1, NW
      VEC(I) = VAL
 10   CONTINUE
C
      RETURN
      END
C
C - - - - - - - - - - - - - -
C
      SUBROUTINE SFVMV (VEC1, VEC2, NW)
      DIMENSION VEC1(1), VEC2(1)
C
C     SFVMV - STANDARD FORTRAN VECTOR MOVE
C
      DO 10 I = 1, NW
      VEC2(I) = VEC1(I)
 10   CONTINUE
C
      RETURN
      END
-----------------------------
          B.IC.NEU
-----------------------------
C
C
```

```
      DO 6000 J = 1, NS
      DO 6000 I = 1, MPSI
      ALPHA(J,I) = 1.0E-60
      IF(J .EQ. JH2O) ALPHA(J,I) = 1.0
C  H2O IS THE THIRD SPECIES:  H, H2, H2O, HO2, H2O2, O, OH, O2, IONS...
 6000 CONTINUE
C
      RETURN
      ENTRY LOCORS
C
C  CHOMPS THRU IT AS IT NEEDS IT -- (SB DRIVEN)
C
 2121 FORMAT(4X,I3,1P10E12.5)
 2122 FORMAT(4X,I3,1X,I7)
 2123 FORMAT(4X,I3,F10.7,1P9E12.5)
      READ(10,2122) MPSI, NSTEP
      READ(10,2123)IET, ETAT, X, XIO, BBO, XIB, PB, DENS, RATEIN, EO, T
      DO 1210 I = 1, LPSI
      READ(10,2121) K, Y(I), PSI(I), ATA(I), H1(I), H2(I), BB(I),
     $                DPDY(I), DINVD(I), R(I), Z(I)
 1210 CONTINUE
      DO 1211 I = 1, MPSI
      READ(10,2121) K, (ALPHA(J,I), J = 1, NS)
 1211 CONTINUE
C
C
      RETURN
      END
-----------------------------
            B.PREP
COMMENT:  ADAPTED FROM SUBPROGRAM WRITTEN BY RIO (AS IN ALPHPREP ABOVE)
-----------------------------
      SUBROUTINE PREP ( RO, RATE )
C
C   ..................................................
C   . H2O VERSION :                 : H2O SPECIES IS NUMBER 15 .
C   ..................................................
C
C
C   NOTE:  RO IS MASS DENSITY IN GM/CC.  DENS IS NUMBER DENSITY IN #/CC
C
      DIMENSION BT(5),DT(5),GM(5),AA(5),YY(19,4),YF(4)
      DIMENSION NJ(25),ISPECF(25),NJJ(25,19),SPEC(25,19)
C
      COMMON/YIELD/ BT,DT,GM,AA,YY,NJ,NJJ,ISPECF,SPEC,YYELEC
C
C
C READ/WRITE OPTION
C
```

```
      N1A=5
      N1B=6
C
C     READ(N1A,207) NS
      NS = 14
C     HARDWIRE THAT IN HERE. DAN'S SPECIES LIST
C     15TH SPECIES, H2O  NEGATIVE YIELD IGNORED IN DAN'S PROGRAM, DIFKT
C     IGNORED IN MINE TOO, BUT NS=14 BECAUSE IGNORED IN HIS
C     N SUB H2O  IS 15.
C
C     SEE SUBROUTINE BOATYI FOR COMPLETE MAPPING BETWEEN
C     HIS SPECIES LISTING AND MINE
C
C
C  CONSTANTS
C
      AVOG=6.023E+23
C
C
      RO3=RO*RO*RO
      AVOGI=1./AVOG
C
C
C   BAKGROUND CONC.(H2O) NOT ALLOWED TO VARY
C
C
C
C  INPUT YIELD INFORMATION
C
C  READ THE INTEGRATED YY VALUES
C
      DO 190 J=1,19
C
      READ(N1A,192) E0,IST,(YY(J,I),I=1,4)
  190 CONTINUE
C
C   READ IN SPATIAL PARAMETERS BT, DT AND GM
C     J=1 HIGH ENERGY PLUME;  J=2,3 MID AND LOW ENERGY PLUME (COALESCED)
C     BUT READ IN DUPLICATE FOR NOW TO MINIMIZE MINOR CHANGES---------
C      J=4  SOURCE TERM   AND J=5  ELECTRON DEPOSITION
C
      READ(N1A,200) (BT(J),J=1,5)
      READ(N1A,200) (DT(J),J=1,5)
      READ(N1A,200) (GM(J),J=1,5)
C
C
      DO 1243 J = 1,5
      AA(J) = DT(J)*BT(J)**3/8./3.141593
      GM(J) = GM(J)*1.795E-7/RO
 1243 CONTINUE
C
```

```
C   MULTIPLY THE DEPOSITION SPECTRUM BY ELECTRON YIELD
      XNO = 1.
      IF(E0 .LE. 12.6) GO TO 1113
      XNO = .5933 + .03228*E0
 1113 CONTINUE
      AA(5) = XNO*AA(5)
C
C-----------------------------------------------------------------------------
C
C READ IN POINTERS FOR PRODUCTION OF VARIOUS SPECIES
C
      DO 209 I=1,NS
C
      READ(N1A,207) NJ(I),ISPECF(I),(NJJ(I,NN),NN=1,19)
      IF(ISPECF(I).EQ.1) READ(N1A,208) (SPEC(I,NN),NN=1,10)
C
  209 CONTINUE
C
      WRITE(N1B,185) E0,NS
C
C
C
C
C WRITE YIELD INPUT
C
      WRITE(N1B,195)
      WRITE(N1B,199)
C
      WRITE(N1B,201) (BT(I),I=1,5)
      WRITE(N1B,202) (DT(I),I=1,5)
      WRITE(N1B,203) (GM(I),I=1,5)
      WRITE(N1B,204) (AA(I),I=1,5)
C
C PROCESS YIELDS
C
       WRITE(N1B,328)
       WRITE(N1B,329)
C
      DO 350 J=1,19
C
      DO 320 I=1,4
C
      YF(I)=YY(J,I)*AVOGI*RATE*RO3
      YF(I)=YF(I)*AA(I)
C
C
  320 CONTINUE
C
      WRITE(N1B,330) (YY(J,I),YF(I),I=1,4)
C
```

```
C
      DO 325 I=1,4
C
      YY(J,I)=YF(I)
  325 CONTINUE
  350 CONTINUE
C
C  ELECTRON NORMALIZATIO
C
C  NOTE A(5) INCLUDES NUM. OF THERMAL ELECTRONS
C
      YYELEC=AA(5)*AVOGI*RATE*RO3
C
C
      DO 400 I=1,5
C
      BT(I)=BT(I)*RO
C
  400 CONTINUE
      WRITE(N1B,498)
      WRITE(N1B,499)
C
      DO 520 I=1,NS
C
      NNMAX=NJ(I)
      WRITE(N1B,500) I,NJ(I),(NJJ(I,NN),SPEC(I,NN),NN=1,NNMAX)
  520 CONTINUE
C
      WRITE(N1B,195)
C
      RETURN
C
C FORMAT STATEMENTS
C
    2 FORMAT(2A4,2X,G12.5,3X,G12.5)
  192 FORMAT(1X,F8.2,2X,I3,1X,4(1X,G14.7))
  200 FORMAT (5G12.5)
  207 FORMAT (22(I2,1X))
  208 FORMAT (10G5.3)
C
  195 FORMAT (' ',//,130('-'))
  199 FORMAT (' ',//,T50,' YIELD INPUT')
C
  185 FORMAT('1',/' ENERGY=',G12.5, 'EV',/,' NUMBER OF SPECIES IS ',
     #I2/1H ,'        (H2O NOT COUNTED)'/)
C
  201 FORMAT(' ' ,//,' BETA ',T15,'::',5(G12.5,2X))
  202 FORMAT(' ' ,/,' DELTA ',T15,'::',5(G12.5,2X))
  203 FORMAT(' ' ,/,' GAMMA',T15,'::',5(G12.5,2X))
  204 FORMAT(' ' ,/,' A-NORM.',T15,'::',5(G12.5,2X))
```

```
C
C
 328   FORMAT(' ',///,T2,'INTEGRATED YIELD; YY INPUT AND YY*FACTORS'/)
 329   FORMAT(' ',T20,'TERMS 1 -> 3 AND SOURCE')
 330   FORMAT(' ',4(G12.5,1X,G12.5,6X))
C
 498   FORMAT (' ',///,' STATES WHICH CONTRIBUTE TO PARTICULAR SPECIES')
 499   FORMAT (' '/,T2,' SPECIES',T11,'#STATES',T30,'STATES AND SPECIAL'
      #,' FACTORS')
 500   FORMAT (' '/,T4,I2,T12,I2,3X,10(I2,1X,F5.3,3X))
C
       END
-----------------------------
            B.YI.HOH
COMMENT:  ADAPTED FROM SUBPROGRAM WRITTEN BY RIO (AS IN ALPHYLDC ABOVE)
-----------------------------
C
      DIMENSION KI(15), IP(15)
C
C
      DIMENSION BT(5),DT(5),GM(5),AA(5),YY(19,4)
      DIMENSION NJ(25),ISPECF(25),NJJ(25,19),SPEC(25,19)
C
      COMMON/YIELD/ BT,DT,GM,AA,YY,NJ,NJJ,ISPECF,SPEC,YYELEC
C
C
C-----------------------------------------------------------------------------
C  6/10/84  ASSIGN B23D = BT(2).  RECALL BT(I) = BT(I)*RO IN SUBR. PREP
C  B23D WILL BE USED THROUGHOUT AS THE DOMINANT FALLOFF PARAMETER IN ORDER
C  TO ASSIGN REDUCED TIMES AND DISTANCES TO CALCULATE XIO, XIE...
C
C     B23D = BT(2)
C  B23D GOES INTO THE UNLABELLED COMMON
C  TOO LATE TO GET IT AT THIS POINT . YOU NEED IT EARLIER SO IT MUST BE
C  READ IN WHERE IT IS INPUTTED 'BY HAND', NAMELY IN SUBR. BOATSA
C-----------------------------------------------------------------------------
C
C
C     DATA KI / 1, 7, 2, 15, 5, 4, 6, 8, 3, 13, 12, 11, 10, 14, 9 /
C     DATA IP / 2*1, 3*0, 3*1, 1*0, 3*1, 3*0 /
C
      DATA KI / 1,6,2,15,10,9,7,5,8,4,14,13,3,11,12 /
      DATA IP / 3*1, 0, 3*1, 5*0, 2*1, 0 /
C
C****  EXPLANATION IS PERHAPS IN ORDER HERE:
C
C        DAN                    MY
C
C   1    1 E        1    1    1  E
C   1    2 H2       1    6    2  H
```

```
C    1    3 H2O+       1    2    3   H2
C    0    4 H3O+       0   15    4   H2O
C    1    5 OH         0   10    5   HO2
C    1    6 H          0    9    6   H2O2
C    1    7 O          1    7    7   O
C    0    8 O2         1    5    8   OH
C    0    9 H2O2       0    8    9   O2
C    0   10 HO2        0    4   10   H3O+
C    0   11 H+(H2O)2   1   14   11   H+
C    0   12 H+(H2O)3   1   13   12   OH+
C    1   13 OH+        1    3   13   H2O+
C    1   14 H+         0   11   14   H+(H2O)2
C        15 H2O        0   12   15   H+(H2O)3
C
C   ON THE LEFT IS DAN'S LIST IN ORDER.  ON THE FAR RIGHT IS MY LIST IN ORDER.
C   MOVING TO THE LEFT FROM MY LIST IS DAN'S CORRESPONDING LIST NUMBER.
C   TO THE LEFT OF THAT IS A 1 OR 0 DEPENDING ON WHETHER THIS SPECIES SHOULD
C   HAVE A NON-ZERO PRIMARY YIELD.  ON THE  F A R  LEFT IS THE LIST OF 1'S AND
C   0'S MAPPING HORIZONTALLY TO DAN'S LIST RATHER THAN TO MINE.  THEREFORE THE
C   ARRAY IP AND ITS USE VIA THE MAPPING ARRAY KI.
C
C   KI GIVES DAN'S LIST NUMBER AS A FUNCTION OF MY LIST NUMBER
C   IP GIVES THE ON-OFF SWITCH AS A FUNCTION OF DAN'S LIST NUMBER
C
C
      CALL SFVFL (0., YI, 2525)
C
C   IN THIS NEUTRAL VERSION WE NEED NOT OMIT THE PSEUDOSPECIES 'DBL'
C
      DO 1500 J = 1, 15
      KIT = KI(J)
      IF(IP(KIT) .EQ. 0) GO TO 1500
C
      DO 1499 I = 1, MPSI
      TAX = R(I)
      TAY = Z(I)
C
      YS=0.0
C
      JMAX=NJ(KIT)
      IF (JMAX.EQ.0) GO TO 14
C
      DO 12 II=1,4
C
      YSADD=0.0
C
      CORREC = DT(II)*DT(II)
      YGEXP=-BT(II)*SQRT(TAX*TAX+CORREC*(TAY-GM(II))*(TAY-GM(II)))
      IF(YGEXP.LT.-150.) GO TO 12
      YG=EXP(YGEXP)
```

```
C
      YSUM=0.0
C
      DO 11 JJ=1,JMAX
C
      YADD=0.0
C
      YADD=YY(NJJ(KIT,JJ),II)
      IF(ISPECF(KIT).EQ.1) YADD=YADD*SPEC(KIT,JJ)
C
      YSUM=YSUM+YADD
C
   11 CONTINUE
C
      YSADD=YG*YSUM
      YS=YS+YSADD
C
   12 CONTINUE
C
      IF(KIT.NE.1) GO TO 13
C  KIT = 1 FOR THE ELECTRON
C
      COREC5 = DT(5)*DT(5)
      YGEXP=-BT(5)*SQRT(TAX*TAX+COREC5*(TAY-GM(5))*(TAY-GM(5)))
      IF (YGEXP.LT.-150.) GO TO 13
      YGELEC=YYELEC*EXP(YGEXP)
C
      YS=YS+YGELEC
C
   13 CONTINUE
C
      GO TO 20
C
   14 CONTINUE
C
      YS=0
C
   20 CONTINUE
C
C-------------------------
      YI(J,I) = YS
C-------------------------
 1499 CONTINUE
 1500 CONTINUE
C
C
C
C
      DO 1600 I = 1, MPSI
      YI(2,I) = YI(2,I) + 1.*YI(12,I) + 2.*YI(11,I) + 1.*YI(13,I)
```

```
C
      YI(8,I) = YI(8,I) + 1.102*YI(12,I) + 1.*YI(11,I) + 1.*YI(13,I)
C
      YI(7,I) = YI(7,I) + .449*YI(12,I)
C
CC    YI(1,I) = YI(1,I) - YI(12,I) - YI(11,I) - YI(13,I)
CC    IF(YI(1,I) .LT. 0.) YI(1,I) = 0.
C  NEVER USED.  ELECTRON CORE DEFICIT TO BE ADDRESSED LATER.
C
C-----------------------------------------------------------
      JH2O = 0
C  REACT H2O.  VERY IMPORTANT.  MASS BALANCE
      YI(4,I) = -YI(7,I) - YI(8,I)
C  THE ELECTRON AFTER RECOMBINATION NETWISE DISSOCIATES H2O TO
C  H + OH AND H2 + O.  THE OH CAN DISSOCIATE TO O + H.
C  H2 TO H + H BUT WE NEED NOT CONCERN WITH IT.
C  NET OH PLUS O PRODJCTION THEN GIVES BACK ORIGINAL SUM.
C
C
 1600 CONTINUE
C
C  2 - H    8 - OH    7 - O    1 - E      12 - OH+    11 - H+    13 - H2O+
C  4 - H2O
C
C
C
C
C
C  DELETE THE ELECTRON FROM THE SPECIES LIST:
C
      JH2O = JH2O - 1
C
      DO 1122 I = 1, MPSI
      DO 1122 J = 1,8
 1122 YI(J,I) = YI(J+1,I)
C
C
C*****************************************************************************
C 10/3/84
C          ADAPT TO H + OH + M --> H2O* + M
C     H - 1  H2O - 2  OH - 3  H2O* - 4          BY H2O* IS MEANT EXC1
C
C*****************************************************************************
      DO 1133 I = 1,MPSI
C     (YI(1,I) = YI(1,I))
      YI(2,I) = 0.
      YI(3,I) = YI(7,I)
      YI(4,I) = 0.
 1133 CONTINUE
C
```

```
C
C
      RETURN
      END
-----------------------------
              A.NR
COMMENT:  GENERALIZED COORDINATE CALCULATION
-----------------------------
      SUBROUTINE BOATNR ( Y, ETAT, BB, Z0, LPSI, R4, Z4, R1, R2, Z1,
     $   ZEE2, H1, H2, ATA4 )
C
C  THE ODD NAME ZEE2 IS THAT WAY SO AS NOT TO CONFLICT WITH Z2 = Z*Z IN
C  NEWTON-RAPHSON MODULE EVEN THOUGH IT HAS BEEN  C O M M E N T E D   O U T
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 Y(101), ETAT, BB(101), Z0, R1(101), R2(101), Z1(101)
      REAL*4 ZEE2(101), H1(101), H2(101), R4(101), Z4(101), SEND(10)
      REAL*4 ATA4(101)
      LOGICAL  L0, L1
C
      DIMENSION XIARR(2001), RHOARR(2001), ZZARR(2001)
      DIMENSION ATA(101), RR(101), ZZ(101)
C  ATA, THE LOCAL ORTHOG. COORD. DOES NOT NEED TO BE KNOWN OUTSIDE OF
C  THIS SUBR.  SO IT IS NOT SENT OUT.
C
C
      COMMON /NRB/ SEND, INR
      COMMON /STORE/ XIARR, RHOARR, ZZARR
C
C$$$
```

```
C
C   INPUTS ARE Y, ETAT, BB, Z0 ----->  XI, ETA, B, Z0
C   OUTPUTS ARE  R1, R2, Z1, Z2, H1, H2,   R, ZZ
C   <---- DRDXI, DRDETA, DZDXI, DZDETA, HXI, HETA,   RHO, Z
C
      ETA = ETAT
      BIG = 1.E30
C
C-----------------------------------------
      SIGN = 1.0D0
      IF(ETA .LT. 0.D0) SIGN = -1.0D0
      ETA = DABS(ETA)
C  (ETA = SIGN*ETA)
C-----------------------------------------
C
      L0 = ETA .LT. 1.D-7
C
      COETA = 1.D0 - ETA
      L1 = COETA .LT. 1.D-7
C
C''''''
```

```
   10 CONTINUE
C
C
C
C
      RHOARR(1) = 0.D0
      XIARR(1) = 0.D0
C
      ETAP = ETA/DSQRT(1.D0 - ETA*ETA)
      NZM1 = NZ - 1
      DO 10014 J = 1,NZM1
      Z = ZZARR(J+1)
C
C
C   CORE REGION >>>>
```

```
      B = 1. + (BB0 - 1.)/(1. + (XIKES/XIB)**PB)
      REL = 1. - B/BSAV
      REL = DABS(REL)
C
C
      IF(REL .LE. 1.E-7) GO TO 78
   77 CONTINUE
      WRITE(6,111)
  111 FORMAT(1H ,'99 ITERATIONS TO EVALUATE B(XI)...................')
   78 CONTINUE
C
      XIARR(J+1) = DSQRT(R*R + Z*Z/B/B)
C
10013 CONTINUE
10014 CONTINUE
C
C---------- --------- ---------- --------- ---------- -------- -----------
C
C  SKIP EULER MODULE IF INR = 1 WHEN ABOUT TO ENTER IT, I.E.
C  COME HERE DIRECTLY AFTER THE FIRST TIME FOR THIS VALUE OF ETA
C
C  INR IN COMMON /NRB/  SHARED WITH SB AND M2 CALLING SUBS
C
10101 CONTINUE
C
      RR(1) = 0.
      ZZ(1) = 0.
      ATA(1) = ETA
C
      DO 902 I = 2, LPSI
      YX = Y(I)
      DO 800 J = 2, NZ
      K = J
      IF(YX .LE. XIARR(J)) GO TO 805
  800 CONTINUE
      WRITE(6,8001) I, Y(I), XIARR(NZ)
 8001 FORMAT('0', I3, 1P2E13.5//)
  805 CONTINUE
C
      RAT = (YX - XIARR(K-1))/(XIARR(K) - XIARR(K-1))
      RR(I) = RHOARR(K-1) + RAT*(RHOARR(K) - RHOARR(K-1))
      ZZ(I) = ZZARR(K-1) + RAT*(ZZARR(K) - ZZARR(K-1))
C
      ATA(I) = ETA
      IF ( ZZ(I) .LE. ZC ) GO TO 903
      ATAP = ZZ(I)**(BB(I)**2)/RR(I)
      ATA(I) = ATAP/DSQRT(1.D0 + ATAP*ATAP)
  903 CONTINUE
  902 CONTINUE
C
```

```
C
 1999 CONTINUE
      DO 2000 I = 1, LPSI
      XI = Y(I)
      B = BB(I)
      IF( L0 ) GO TO 9991
      IF( L1 ) GO TO 9992
C     IF XI = 0. GO TO 9992      Y(1) = 0.,  THEREFORE
      IF ( I .EQ. 1 ) GO TO 9992
C  BY THE WAY, WHEN YOU GET THERE, DON'T FORGET TO SEPARATELY
C  DEFINE TATA TO BE ATA(1)
C
      TATA = ATA(I)
C
C  REPLACING THE GLOBAL CANONICAL FORM WITH THE LOCAL ADIABATIC ONE.
C  CHANGE A MINIMUM OF SYMBOLOLOGY
C
C     ETA2 = ETA*ETA  REPLACED BY
C
      ETA2 = TATA*TATA
      ETAP = TATA/DSQRT(1.D0 - ETA2)
C
      B2 = B*B
      B4 = B2*B2
      RB2 = 1.D0/B2
      RB4 = 1.D0/B4
C
      XI2 = XI*XI
C
C
      ETAP2 = ETAP*ETAP
      ETPRB2 = ETAP**RB2
C
      GSIN = DSQRT(1.D0 - ETA2)
C
C  D(ETAP)/DETA =
      DETPDE = 1./GSIN**3
C
C  D(ETPRB2)/DETA =
      DERBDE = RB2*ETPRB2/ETAP*DETPDE
C
      ETA2B2 = ETA2**RB2
      COMPB2 = 1.D0 - ETA2B2
C
C
C
C  NEWTON-RAPHSON CONVERGENCE CALCULATION OF RHO AND Z
C
C     COEFF = ETAP2**RB2/B2
C     NEVER USED
```

```
C
C=====================================================================
C   DELETE NEWTON-RAPHSON
C=====================================================================
CC INITIAL ESTIMATE - UPPER BOUND
C
C       EZ21 = B2*XI2
C       EZ22 = (ETAP2*XI2)**RB2
C       EZ2 = DMINI(EZ21,EZ22)
C
CC NEWTON-RAPHSON CONVERGENCE ON ZERO
CC NOTE: F(Z2) IS CONCAVE UPWARD - WELL ADAPTED FOR THE N-R TECHNIQUE
C
CC F(Z2) = Z2**B2/ETAP2 + Z2/B2 - XI2
C
C       N = 1
C       Z2 = EZ2
C       DO 1000 M = 1, 99
C       FF = Z2**B2/ETAP2 + Z2/B2 - XI2
C       FFP = B2*Z2**(B2-1.)/ETAP2 + RB2
C       Z2P = Z2 - FF/FFP
C       REL = 1. - Z2P/Z2
C       REL = DABS(REL)
C  ABS. VAL. NOT ACTUALLY NECESSARY
C       Z2 = Z2P
C       IF(REL .LT. 1.D-14) GO TO 1001
C       N = N + 1
C1000 CONTINUE
C       WRITE(6,*)   REL
C1001 CONTINUE
C       Z = DSQRT(Z2)
C       RHO = Z**B2/ETAP
C=====================================================================
C
C   INCORPORATE EULER RESULTS
C
        Z = ZZ(I)
        RHO = RR(I)
C
C
C
 9990 CONTINUE
C
C
C
        Z2B2 = Z**(2.0D0*B2)
        ER = ETAP*RHO
        ER2RB2 = ER**(2.0*RB2)
C
C* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
```

```
C
C       WRITE(6,*) B, B2, B4, RB2, RB4, ETA, ETA2, ETAP, ETAP2
C       WRITE(6,*) Z, RHO, Z2B2, ER, ER2RB2, XI, I, Y(I)
C
C  3. PARTIALS CALCULATED BY IMPLICIT DIFFERENTIATION.  RHO AND Z  CALCULATED
C     BY NEWTON-RAPHSON TECHNIQUE.
C
C
      DZDXI = XI/(B2*Z2B2/Z/ETAP2 + Z/B2)
C
      DZDETA = Z2B2/ETAP/ETAP2/(B2*Z2B2/Z/ETAP2 + Z/B2)
      DZDETA = DZDETA*DETPDE
C
      DRDXI = XI/(RHO + RB4*ER2RB2/ER*ETAP)
C
      DRDETA = -RB4*ER2RB2/ER*RHO/(RHO + RB4*ER2RB2/ER*ETAP)
      DRDETA = DRDETA*DETPDE
C
      HXI = DSQRT(  DRDXI**2  +  DZDXI**2  )
      HETA = DSQRT(  DRDETA**2  +  DZDETA**2  )
C
      GO TO 9993
 9991 CONTINUE
C     IF (LO) COME HERE
C
C
      RHO = XI
      Z = 0.D0
      TATA = 0.D0
      DRDXI = 1.D0
      DRDETA = 0.D0
      DZDXI = 0.
      DZDETA = BIG
C
C     DZDETA --- RB2*(XI*ETA)**(RB2-1.D0)*XI  AS ETA --> 0.
C  (AS ETA -->  0.   Z  ---  (XI*ETA)**(1/B**2)
C
      HXI = 1.D0
      HETA = BIG
C
C
      GO TO 9993
C
 9992 CONTINUE
C   IF(L1) COME HERE
C
C
      RHO = 0.D0
      Z = XI*B
```

```
      TATA = 1.D0
      IF(.NOT.L1) TATA = ATA(1)
      DRDXI = 0.D0
      DRDETA = -BIG
      DZDXI = B
      DZDETA = 0.D0
C
C  DRDXI --> + INFINITY AS ETA --> +/- 1
C
      HXI = B
      HETA = BIG
C
 9993 CONTINUE
C-----------------------------------------------------------------
      IF(SIGN .EQ. 1.D0) GO TO 999
      ETA = -ETA
C  RE-ESTABLISH ETA  ARGUMENTS ARE INPUTS-OUTPUTS, REMEMBER...
      Z = -Z
      TATA = -TATA
      DRDETA = -DRDETA
      DZDXI = -DZDXI
  999 CONTINUE
C-----------------------------------------------------------------
C
C
      R4(I) = RHO
      Z4(I) = Z + Z0
C     Z4(I) = Z
      R1(I) = DRDXI
      R2(I) = DRDETA
      Z1(I) = DZDXI
      ZEE2(I) = DZDETA
      H1(I) = HXI
      H2(I) = HETA
      ATA4(I) = TATA
 2000 CONTINUE
C
C2222 FORMAT(1H0,'NR-----NR-----NR-----NR-----NR'/)
C2223 FORMAT(1H0)
C2224 FORMAT(1H ,1P10E12.5)
C2225 FORMAT(1H ,1P10D12.5)
C     WRITE(6,2222)
C     WRITE(6,2223)
C     WRITE(6,2224) (R4(I),I=1,LPSI)
C     WRITE(6,2224) (Z4(I),I=1,LPSI)
C     WRITE(6,2224) (ATA4(I),I=1,LPSI)
C     WRITE(6,2223)
C     WRITE(6,2225) (XIARR(I),I=1,1001)
C     WRITE(6,2225) (RHOARR(I),I=1,1001)
C     WRITE(6,2225) (ZZARR(I),I=1,1001)
```

```
C     WRITE(6,2222)
C
C
      RETURN
      END
-----------------------------
            UT.SMBBL
COMMENT:  SIMPSON'S RULE INTERPOLATION SUBROUTINE WITH BUBBLE SEARCH
-----------------------------
      SUBROUTINE SIMSON (X, F, XI, FI, N, M, IC)
C
C  THIS SUBROUTINE INTERPOLATES USING SIMPSON'S RULE (PARABOLIC INTERPOL-
C  ATION) BETWEEN DATA POINTS ( X(I), F(I) ) TO PRODUCE INTERPOLATED POINTS
C  ( XI(J), FI(J) ).  X MUST BE IN ASCENDING ORDER WITH NO REDUNDANT POINTS.
C
C  ARRAYS X(I) AND F(I), I = 1, N
C         XI(J) AND FI(J), J = 1, M
C
C  DEFAULT INTERPOLATION:  IF IC = 0 THEN DEFAULT SET XI(J) EQUALLY SPACED
C  BETWEEN X(1) AND X(N) IS IMPLEMENTED.
C
C  IF IC = 1 THEN XI IS INPUTTED IN THE SUBROUTINE CALL
C
C
      DIMENSION X(1), F(1), XI(1), FI(1)
      DIMENSION A(22), B(22), C(22)
C
C
      NM1 = N - 1
      NM2 = N - 2
      DO 10 I = 1, NM2
      X1 = X(I)
      X2 = X(I+1)
      X3 = X(I+2)
      F1 = F(I)
      F2 = F(I+1)
      F3 = F(I+2)
      X1Q = X1*X1
      X2Q = X2*X2
      X3Q = X3*X3
      F1Q = F1*F1
      F2Q = F2*F2
      F3Q = F3*F3
C
      DET = X2*X1Q + X1*X3Q + X3*X2Q - X1Q*X3 - X3Q*X2 - X2Q*X1
      IF(DET .EQ. 0.E0) GO TO 101
C
      DEA = X2*F1  + X1*F3  + X3*F2  - F1 *X3 - F3 *X2 - F2 *X1
      DEB = F2*X1Q + F1*X3Q + F3*X2Q - X1Q*F3 - X3Q*F2 - X2Q*F1
```

```
C
      DEC = X2*X1Q*F3 + X1*X3Q*F2 + X3*X2Q*F1 - X1Q*X3*F2 - X3Q*X2*F1
     $        - X2Q*X1*F3
C
      A(I) = DEA/DET
      B(I) = DEB/DET
      C(I) = DEC/DET
      GO TO 102
C
  101 CONTINUE
      A(I) = 0.
      B(I) = (F2 - F1)/(X2 - X1)
      C(I) = F1 - X1*B(I)
C
  102 CONTINUE
C
   10 CONTINUE
C
      A(NM1) = A(NM2)
      B(NM1) = B(NM2)
      C(NM1) = C(NM2)
C
C
C     WRITE(6,*) A,B,C
      DO 11 I = 2, NM2
      A(I) = (A(I-1) + A(I))/2.
      B(I) = (B(I-1) + B(I))/2.
      C(I) = (C(I-1) + C(I))/2.
   11 CONTINUE
C     WRITE(6,*) A,B,C
C
      IF ( IC .EQ. 1) GO TO 200
C
C  DEFAULT INTERPOLATION POINTS
C
      DELTA = (X(N) - X(1))/(M - 1)
      XI(1) = X(1)
      DO 20 I = 2, M
   20 XI(I) = XI(I-1) + DELTA
C
  200 CONTINUE
C
C  I WILL NOT BOTHER TO PUT A CHECK HERE THAT X(1) .LE. XI(J) .LE. X(N),
C  J = 1, M   IN CASE THE XI(J) ARE INPUTTED.
C
C
C  BUBBLE SEARCH FOR ASCENDING XI
C
      K = 2
      DO 40 J = 1, M
```

:

```
      XJ = XI(J)
C  FIND I SUCH THAT XI(J) .LE. X(I).  IN THIS EVENT X(I-1) .LT. XI(J) FOR
C  I .GT. 2 AND .LE. XI(J) FOR I .EQ. 2
C
      DO 35 I = K, N
      KK = I
      IF(XJ .LE. X(I)) GO TO 36
   35 CONTINUE
   36 CONTINUE
      K = KK
      FI(J) = A(KK-1)*XJ**2 + B(KK-1)*XJ + C(KK-1)
C  BINS INDEXED FROM BELOW
   40 CONTINUE
C
C
      RETURN
      END
-----------------------------
              B.CC
-----------------------------
C
C
      LOGICAL L510
C
C
      SIGN = 1.0
      L510 = (K/5)*5 .EQ. K
      DO 100 J = 1, NJ
      IF (J .GT. 2) SIGN = -1.0
      IROW = IRRR(I,J)
      IF (J.EQ.2 .AND. L510) IROW = NSX
        DO 80 IEQ = 1, NEQ
          GO TO (10, 20, 30, 40, 50), IEQ
 10       IF (L510) GO TO 15
          IF (ALPHA(J1,L).EQ. 0.0) GO TO 80
          TEMP = SIGN*TEMRP/ALPHA(J1,L)
          GO TO 60
 15       TEMP = SIGN*CRR
          GO TO 60
 20       IF (L510) GO TO 80
          IF (ALPHA(J2,L).EQ. 0.0) GO TO 80
          TEMP = SIGN*TEMRP/ALPHA(J2,L)
          GO TO 60
 30   CONTINUE
          IF (ALPHA(J3,L).EQ.0.0) GO TO 80
          TEMP = -SIGN*TEMRM/ALPHA(J3,L)
          GO TO 60
 40   CONTINUE
          IF (ALPHA(J4,L).EQ.0.0) GO TO 80
          TEMP = -SIGN*TEMRM/ALPHA(J4,L)
```

```
          GO TO 60
 50     CONTINUE
            IF (ALPHA(J5,L).EQ. 0.0) GO TO 80
            TEMP = -SIGN*TEMRM/ALPHA(J5,L)
 60         IJ = J12345(IEQ)
            CM(IROW,IJ) = CM(IROW,IJ) + TEMP
 80       CONTINUE
        IF (K.EQ. 10) GO TO 100
        IF (K .EQ. 5) GO TO 85
        QX(IROW) = QX(IROW) + QSIGN*SIGN*(TEMRP + RMFAC*TEMRM)
        GO TO 100
 85     QX(IROW) = QX(IROW) + QSIGN*SIGN*TEMRM
 100    CONTINUE
        RETURN
        END
-----------------------------
              B.EF
-----------------------------
C
C
        E = 0.0
        SIGN = 1.0
        DO 10 N = 1, NJ
        IF (N.EQ.2 .AND. K.EQ.5) GO TO 10
        IF (N.GT.2) SIGN = -1.0
        J = J12345(N)
        E = SIGN*G(J) + E
 10     CONTINUE
C
        E = E/RRT
        IF(ABS(E) .LT. 80.) GO TO 20
        IF(E. LT. 0.) GO TO 25
        IF(E .GT. 0.) E = EXP(80.)
        GO TO 30
 25     E = EXP(-80.)
        GO TO 30
 20     E = EXP(E)
 30     BOATEF = E
        RETURN
        END
-----------------------------
           A.S2DKED
-----------------------------
C
C
        LOGICAL OUT
C
        FACTR = 1.
        RR = 1.987
C
```

```
C   ALERT ALERT UNITS.....CHANGE RR TO CGS-CAL UNITS.    NOW @@@@@@
C
C   CHANGE R TO RR SO AS NOT TO CONFLICT WITH THE RADIAL COORDINATE ARRAY
C
C   ESTHETIC SACRIFICE.
C
C
      AV = 6.0225E23
      OUT = .FALSE.
      DO 899 L=1,NPSI
C   THIS IS THE NEW SYSTEM: EXTRAPOLATE THE EDGE POINT, DO NOT EXTRAPOLATE
C   THE PROPAGATION OF THE EDGE POINT, I.E. DO NOT PROPAGATE IT DIRECTLY,
C   RATHER, INDIRECTLY ON THE BASIS OF EXTRAPOLATION
C
C
C   NOTE: FOR THE RADIOLOGICAL APPLICATION WE MUST ALSO TAKE INTO
C   ACCOUNT DIFFUSION AND CHEMICAL EVOLUTION AT THE EDGE
C
      CALL SFVFL(0.0, QX, NSX)
      IF( NR .EQ. 0 ) GO TO 3256
      RRT=1.986*T
      ROOTT=SQRT(T)
      TX=T
      CALL SFVFL (0.0, WP, NSX)
      CALL SFVFL (0.0, WM, NSX)
      NSX2=NSX**2
      CALL SFVFL (0.0, CM, NSX2)
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CCC    IF(T-TKINET) 3256,3256,3259
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
 3259 CONTINUE
C
C
      DO 862 I=1,NR
      TEMRP=0.0
      TEMRM=0.0
      KK = IRT(I)
C
C     REACTION CONSTANT TYPE
C
      GO TO (841,842,843,844,845,846,847,848),KK
  841 RATE=RC(I,1)*AV
      GO TO 849
  842 RATE=RC(I,1)/T*AV
      GO TO 849
  843 RATE=RC(I,1)/T/T*AV
      GO TO 849
  844 RATE=RC(I,1)/ROOTT*AV
```

```
      GO TO 849
  845 RATE=RC(I,1)*EXP(RC(I,3)/RRT)*AV
      GO TO 849
  846 RATE=RC(I,1)*EXP(RC(I,3)/RRT)/T*AV
      GO TO 849
  847 RATE=RC(I,1)/T/ROOTT*AV
      GO TO 849
  848 RATE=RC(I,1)*EXP(RC(I,3)/RRT)/(T**RC(I,2))*AV
  849 CONTINUE
C
C-------------------------------
C  MULTIPLY RATE BY 1/RHO
C
      RATE = RATE/RO
C-------------------------------
C
      K=IRR(I)
C
C     TYPE OF REACTION
C
      DO 100 N = 1, 5
 100  J12345(N) = IRRR(I,N)
      GO TO(864,865,866,870,871,834,835,836,837,838),K
 870  CONTINUE
      E = BOATEF (K, 3, RRT)
       CRR=RATE*RO/FACTR
      TEMRP=CRR*RO/FACTR*ALPHA(J1,L)*ALPHA(J2,L)
      TEMRM=CRR*ALPHA(J3,L)/E/RR/T
      CALL BOATCC (K, I, L, 3, 3, 1.0, 0.0)
      GO TO 868
 871  CONTINUE
      J2=NSX
      E = BOATEF (K, 4, RRT)
       CRR=RATE*RO/FACTR*RO/FACTR/WTMIX
      TEMRP=CRR*ALPHA(J1,L)
      TEMRM=CRR*RR*T*RO/FACTR*ALPHA(J3,L)*ALPHA(J4,L)/E
      CALL BOATCC (K, I, L, 4, 4, -1.0, 0.0)
      GO TO 867
 864  CONTINUE
      E = BOATEF (K, 4, RRT)
       CRR=RATE*RO/FACTR*RO/FACTR
      TEMRP=CRR*ALPHA(J1,L)*ALPHA(J2,L)
      TEMRM=CRR*ALPHA(J3,L)*ALPHA(J4,L)/E
      CALL BOATCC (K, I, L, 4, 4, 1.0, -1.0)
      GO TO 867
 865  CONTINUE
      E = BOATEF (K, 3, RRT)
       CRR=RATE*RO/FACTR*RO/FACTR/WTMIX*AV
      TEMRP=CRR*RO/FACTR*ALPHA(J1,L)*ALPHA(J2,L)
      TEMRM=CRR*ALPHA(J3,L)/E/RR/T
```

```
      CALL BOATCC (K, I, L, 3, 3, 1.0, 0.0)
      GO TO 868
 866  CONTINUE
      E = BOATEF (K, 5, RRT)
       CRR=RATE*RO/FACTR*RO/FACTR
      TEMRP=CRR*ALPHA(J1,L)*ALPHA(J2,L)
      TEMRM=CRR*ALPHA(J3,L)*ALPHA(J4,L)*ALPHA(J5,L)*RO
     #        /FACTR*RR*T/E
      CALL BOATCC (K, I, L, 5, 5, 1.0, -2.0)
      GO TO 861
 837  CONTINUE
       CRR=RATE*RO/FACTR
      TEMRP=CRR*RO/FACTR*ALPHA(J1,L)*ALPHA(J2,L)
      TEMRM=0.0
      CALL BOATCC (K, I, L, 3, 2, 1.0, 0.0)
      GO TO 868
 838  CONTINUE
      J2=NSX
       CRR=RATE*RO/FACTR*RO/FACTR/WTMIX
      TEMRP=CRR*ALPHA(J1,L)
      TEMRM=0.0
      CALL BOATCC (K, I, L, 4, 1, 1.0, 0.0)
      GO TO 867
 834  CONTINUE
       CRR=RATE*RO/FACTR*RO/FACTR
      TEMRP=CRR*ALPHA(J1,L)*ALPHA(J2,L)
      TEMRM=0.0
      CALL BOATCC (K, I, L, 4, 2, 1.0, 0.0)
      GO TO 867
 835  CONTINUE
       CRR=RATE*RO/FACTR*RO/FACTR/WTMIX*AV
      TEMRP=CRR*RO/FACTR*ALPHA(J1,L)*ALPHA(J2,L)
      TEMRM=0.0
      CALL BOATCC (K, I, L, 3, 2, 1.0, 0.0)
      GO TO 868
 836  CONTINUE
       CRR=RATE*RO/FACTR*RO/FACTR
      TEMRP=CRR*ALPHA(J1,L)*ALPHA(J2,L)
      TEMRM=0.0
      CALL BOATCC (K, I, L, 5, 2, 1.0, 0.0)
C
C     CALCULATE WDOT
C
 861  WP(J5)=WP(J5)+TEMRP
      WM(J5)=WM(J5)+TEMRM
 867  WP(J4)=WP(J4)+TEMRP
      WM(J4)=WM(J4)+TEMRM
 868  WP(J3)=WP(J3)+TEMRP
      WM(J3)=WM(J3)+TEMRM
      WP(J2)=WP(J2)+TEMRM
```

```
      WM(J2)=WM(J2)+TEMRP
      WP(J1)=WP(J1)+TEMRM
      WM(J1)=WM(J1)+TEMRP
 3254 IF (IREAC .LE. 0) GO TO 862
      IF (IFINIS .EQ. 0) GO TO 500
      IF (X .GE. XMAX) GO TO 500
      IF (PCNT .NE. 0.) GO TO 862
 500  NREC = (L-1)*NRX + I
       CALL SFVMV ( TEMRP, RPRM(NREC), 2 )
      OUT = .TRUE.
  862 CONTINUE
 3256 CONTINUE
      CALL BOATS3(L)
  899 CONTINUE
C
      IF ( OUT )  CALL BOAT02
C
      RETURN
      END
-----------------------------
            B.CHM
COMMENT:  EXTERNALLY SUPPLIED "CHEMISTRY FRIENDLY" TIME STEP
-----------------------------
C
C
C*******************************************************************************
C
C  XCHK EQUALS ONE HALF OF X-INTERSECT ( X - IGNITION )
C  XCHK IS ASSIGNED IN BOATSA.  INPUTED AS CCHM
C
      XCHK = CCHM
C
      CHEM = 0.1*CAS
      IF(CAS .GE. XCHK) CHEM = 0.1*XCHK
      RETURN
      END
-----------------------------
           A.M2DKNM
-----------------------------
C
C  PSION IS ACRONYMIC FOR PSI-OLD/NEW: OLD Y'S.  NEW XIO
C
C
C*****************************************************************
C     DIMENSION PSISAV(101), YSAV(101)
C*****************************************************************
C
      DIMENSION PSION(101), BUF1(101), BUF2(101)
      REAL*8 XIARR(2001), RHOARR(2001), ZZARR(2001)
C
```

```
      DIMENSION SEND(10)
C
      COMMON /NRB/ SEND, INR
      COMMON /STORE/ XIARR, RHOARR, ZZARR
C
C
      SEND(1) = BB0
      SEND(2) = XI0
      SEND(3) = PB
      SEND(5) = XIEDGE
C
C
C
      IFINIS=1
C
C      CHECK FOR NEGATIVE MOLE FRACTION
C
      DO 967 I=1,MPSI
      DO 967 J=1,NS
      DUM=RALPHA(J,I)
      IF(DUM.LT.-1.E-10) GO TO 995
      IF(DUM .LT. 1.E-65) RALPHA(J,I)=1.E-65
  967 CONTINUE
      DFDL=1.
C
C
C
      X=X+DX
      PCNT=PCNT+DX
      NSTEP = NSTEP + 1
C
C
C
C     MAIN INTERPOLATION LOOP
C
C
C
      IF (IINT .EQ. 0) GO TO 333
      IF (MPSI .EQ. 1) GO TO 333
C  GUARANTEE IT.
C
C  PSII IS FIXED AS 0. AS LONG AS XI PRIME = LOG(XI/XI0+1)
C  PSI = XI PRIME.  Y = XI.
      PSII = 0.
C
C
C
C  EVALUATE NEW XI0 = XI0( NEW X = X + DX ) HERE - - - - - - - - - - - - -
C
      XI0SAV = XI0
```

```
C-.-.-.
```

```
      Y(I) = XI0*(EXP((I-1)*DELPSI) - 1.)
      DPDY(I) = 1./(Y(I) + XI0)
      DINVD(I) = -DPDY(I)
      BB(I) = 1. + (BB0 - 1.)/(1. + (Y(I)/XIB)**PB)
C
C
  901 CONTINUE
C
      Y(MPSI) = XIEDGE
C   EXACT TO BE SURE.  NOT JUST LIMIT OF PRECISION OF CALCULATION.
C
C
C     WRITE(6,*) YSAV
C     WRITE(6,10000)
10000 FORMAT(1H0)
C     WRITE(6,*) Y
C
C     WRITE(6,*) PSISAV
C     WRITE(6,10000)
C     WRITE(6,*) PSION
C     WRITE(6,10000)
C     WRITE(6,*) PSI
C
C
C
C   OK...   THERE'S THE NEW GRID.
C
C   OLD VALUES OF XI0, DELPSI  ARE GONE  NOW.
C
C
C~~~
```

```
C       WRITE(6,2224) (ATA(I),I=1,LPSI)
C       WRITE(6,2223)
C       WRITE(6,2225) (XIARR(I),I=1,2001)
C       WRITE(6,2225) (RHOARR(I),I=1,2001)
C       WRITE(6,2225) (ZZARR(I),I=1,2001)
C       WRITE(6,2222)
C
C
C
C-----------------------------------------------------------
        DO 10 I = 1, LPSI
C     COORDINATE TRANSFORMATION : XI --> XI PRIME
C
C   XI PRIME = LN ( XI/XI0 + 1 )
C
        R1P(I) = R1(I)/DPDY(I)
        Z1P(I) = Z1(I)/DPDY(I)
        H1P(I) = H1(I)/DPDY(I)
C
        A(I) = H2(I)*R(I)/H1P(I)
        TRIP(I) = H1P(I)*H2(I)*R(I)
C
C   H1 VARIES FROM 1 AT ETA = 0 TO B AT ABS(ETA) = 1
   10 CONTINUE
C-----------------------------------------------------------
C
C       COMPUTE THE YIELDS
C
        CALL BOATYI
C
C
C~~~
```

```
C
      DO 1162 J=1,NS
      ALPHA(J,I) = RALPHA(J,I)
      IF(J .EQ. JH2O) GO TO 1162
C
      ANORM = RALPHA(J,1)
      DO 1160 I = 1, MPSI
 1160 BUF1(I) = ALOG(RALPHA(J,I)/ANORM)
C
C     WRITE(6,*) BUF1
C     WRITE(6,10000)
C
      CALL SIMSON( PSION, BUF1, PSI, BUF2, MPSI, MPSI, 1 )
C
C     WRITE(6,*) BUF2
C     WRITE(6,10000)
C     WRITE(6,10000)
C
      DO 1161 I = 1, MPSI
      ALPHA(J,I) = ANORM*EXP(BUF2(I))
 1161 CONTINUE
C
 1162 CONTINUE
C
C
C
C
      GO TO 334
  333 CONTINUE
C
C
                                DO 969 I=1,MPSI
                                DO 970 J=1,NS
  970                       ALPHA(J,I)=RALPHA(J,I)
  969                       CONTINUE
C
C
  334 CONTINUE
C
C
C
C   RECALL THAT WORKING UNITS ALPHA = MOLE FRACTION / MIXTURE MOLEC. WT. =
C   MOLAR DENSITY / MIXTURE MASS DENSITY.
C
C   INPUT/OUTPUT UNITS ALPHA = MOLE FRACTION.
C
C
C*****************************************************************
      IF(IDIAG.EQ.0) GO TO 8451
      WRITE(6,8448)
```

```
 8448 FORMAT(1H0//,' BEGIN OF M2-END'//)
      DO 849 I = 1, MPSI
      WRITE(6,8449) (ALPHA(J,I),J=1,NS)
      WRITE(6,8449) (RALPHA(J,I),J=1,NS)
  849 CONTINUE
 8449 FORMAT(1H ,1P8E14.5)
      WRITE(6,8450)
 8450 FORMAT(1H ,' END OF M2-END'///)
 8451 CONTINUE
C*****************************************************************
C
C
      GO TO 6
C
 995  CONTINUE
      WRITE(6,8004) I, J, X, DX, FDL, ALPHA(J,I), RALPHA(J,I)
 8004 FORMAT(24H SPECIES NEGATIVE IN M2%2I5,5E13.5)
      IF (DX .LT. DXMIN) GO TO 8000
      DX = DX/2.0
      FDL=FDL/2.
      NT = NT + 1
      NSTEP = NSTEP + 1
      GO TO 6
C
C
 8000  WRITE(6,8001)
 8001 FORMAT(56HINEGATIVE PARAMETER - NOT CORRECTED BY REPEATED HALVING
     1,12HOF STEP SIZE)
      WRITE(6,8002) I,J,X,Y(I),PSI(I),ALPHA(J,I),RALPHA(J,I)
 8002 FORMAT(2I5,8E13.5)
      STOP
C
C
 6    RETURN
      END
-----------------------------
            B.S3DK
-----------------------------
C
C  SHOULD NOT COME HERE IF L = MPSI
C  UNLESS MPSI = 1 (PURE KINETIC RUN)
C
      DIMENSION DIF(25)
C
C
      I = L
      DP = DPDY(I)
      DI = DINVD(I)
      B = BB(I)
C
```

```
      IF(I.EQ.1) GO TO 800
C
      DUMS = TRIP(I)*DELPSI**2
      AP=.5*(A(I)+A(I+1))
      AM=.5*(A(I)+A(I-1))
C
C
C
      DO 41 J=1,NS
      DIF(J) = 0.
      IF(J .EQ. JH2D) QX(J) = ALPHA(J,I)
      IF(J .EQ. JH2D) GO TO 41
      QX(J) = ALPHA(J,I) + QX(J)*DX
C
C
      ABSETA = ABS(ETAT)
      IF(ETAT .EQ. 0. .OR. ABSETA .EQ. 1.) GO TO 1001
C
      DALFAP = BETA(J,I+1) - BETA(J,I)
      DALFAM = BETA(J,I) - BETA(J,I-1)
      DIF(J) = (AP*DA_FAP - AM*DALFAM)/DUMS*DFCOEF(J)
C
      GO TO 33
 1001 CONTINUE
C
C  FIRST AND SECOND DERIVATIVES WITH RESPECT TO PSI = XI'
      DADP = (BETA(J,I+1) - BETA(J,I-1))/2./DELPSI
      D2ADP2 = (BETA(J,I+1) - 2.*BETA(J,I) + BETA(J,I-1))/DELPSI**2
C
C  ASSIGN COEF1 AND COEF2
C  DEPENDING ON WHETHER ETA = 0 OR ETA = +/- 1
      IF(ABSETA .EQ. 1.) GO TO 1010
C  IF ETA = 0 COME HERE
      COEF1 = 1.
      COEF2 = 1. + 1./B/B
      GO TO 1011
 1010 CONTINUE
C  IF ETA = +/- 1 COME HERE
      COEF1 = 1./B/B
      COEF2 = 2.
 1011 CONTINUE
C
C
      DIF(J) = DFCOEF(J)*(COEF1*DP*(DI*DADP + DP*D2ADP2) + COEF2*DP*
     1  DADP/Y(I))
C
C
   33 CONTINUE
C
   41 CONTINUE
```

```
      IF(NR.EQ.0) GO TO 7811
      DO 781 M=1,NS
      DO 781 N=1,NS
      CM(M,N)= CM(M,N)*DX
      IF (M.EQ.N) CM(M,N)=CM(M,N) +1.0
  781 CONTINUE
      CALL BOATSL(QX,CM,NS)
 7811 DO 782 J=1,NS
  782 RALPHA(J,I)= QX(J) + YI(J,I)*DX/RO + DIF(J)*DX
C
 8000 CONTINUE
C
      GO TO 900
  800 CONTINUE
      IF ( PSI(1).GT.0. )  GO TO 850
C
C
      DO 200 J=1,NS
      DIF(J) = 0.
      IF(J .EQ. JH20) QX(J) = ALPHA(J,1)
      IF(J .EQ. JH20) GO TO 200
      QX(J) = ALPHA(J,1) + QX(J)*DX
C
      IF(MPSI .EQ. 1) GO TO 500
C   PURE KINETIC RUN, SKIP DIFFUSION CALCULATION
C
      IF(ETAT .NE. 0.) GO TO 2010
C   IF ETA = 0 COME HERE
      COEF1 = 1.
      COEF2 = 1. + 1./B/B
      GO TO 2011
 2010 CONTINUE
C   IF ETA =/= 0  COME HERE
      COEF1 = 1./B/B
      COEF2 = 2.
 2011 CONTINUE
C
      DP = (DP + DPDY(2))/2.
      DI = (DI + DINVD(2))/2.
      PSHALF = PSI(2)/2.
C
C   Y(1) = 0     PSI(1) = 0.
C
      YHALF = XI0*(EXP(PSHALF) - 1.)
C
C   NOW USE THIRD DIFFERENCE EXTRAPOLATION TO EXTRAPOLATE D2ADP2.
C
      DADP = (BETA(J,2) - BETA(J,1))/DELPSI
C
      D2A1 = (BETA(J,1) - 2.*BETA(J,2) + BETA(J,3))/DELPSI**2
```

```
      D2A2 = (BETA(J,2) - 2.*BETA(J,3) + BETA(J,4))/DELPSI**2
C
      D2ADP2 = 1.5*D2A1 - 0.5*D2A2
C
C
      DIF(J) = DFCOEF(J)*(COEF1*DP*(DI*DADP + DP*D2ADP2) + COEF2*DP*
     1  DADP/YHALF)
C
  500 CONTINUE
  200 CONTINUE
C
      IF(NR.EQ.0) GO TO 7812
      DO 783 M=1,NS
      DO 783 N=1,NS
      CM(M,N)= CM(M,N)*DX
      IF (M.EQ.N) CM(M,N)=CM(M,N) +1.0
  783 CONTINUE
      CALL BOATSL(QX,CM,NS)
 7812 DO 784 J=1, NS
  784 RALPHA(J,1)= QX(J) + YI(J,1)*DX/RO + DIF(J)*DX
      GO TO 900
  850 CONTINUE
C
C  YOU SHOULD NOT COME HERE. Y(1) SHOULD = 0., SO SHOULD PSI(1).
C
  900 CONTINUE
C
C
      RETURN
      END
-----------------------------
            B.GXDK
-----------------------------
      TX=T
      M=1
      FACTOR=1.98718*TX
      IF(TX.LT.1000.) M=8
C
      DO 100 J=1,NS
      GX=CON(M,J)*(1.-ALOG(TX))-CON(M+1,J)*TX/2.-CON(M+2,J)*
     1TX**2/6.-CON(M+3,J)*TX**3/12.-CON(M+4,J)*TX**4/20.+
     2CON(M+5,J)/TX-CON(M+6,J)
  100 G(J)=GX*FACTOR
C
      RETURN
      END
-----------------------------
            A.INDK
-----------------------------
C
```

```
C
      DIMENSION RPRMV(10)
C
C
      IF(IIN .NE. 0) GO TO 163
      IF(IET .GT. 1) GO TO 161
       WRITE(6,1901)
       WRITE(6,1902) (TITLE(I),I=1,18)
C
      WRITE(6,1908) X,XMAX
       WRITE(6,1916)
C
C
      DO 1919 J=1,NS
      RALPHA(J,1)=ALPHA(J,1)*WTMIX
      RALPHA(J,MPSI)=ALPHA(J,MPSI)*WTMIX
 1919  WRITE(6,1917)AID(J),RALPHA(J,1),RALPHA(J,MPSI)
C
C  RECALL THAT WORKING UNITS ALPHA = MOLE FRACTION / MIXTURE MOLEC. WT. =
C  MOLAR DENSITY / MIXTURE MASS DENSITY.
C
C  INPUT/OUTPUT UNITS ALPHA = MOLE FRACTION.
C
C
      IF(NR.LE.0) GO TO 160
       WRITE(6,120)
      DO 159 I=1,NR
      L=IRR(I)
      GO TO(131,132,133,134,135,136,137,138,139,140),L
  131 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
       WRITE(6,121)I,AID(J1),AID(J2),AID(J3),AID(J4),
     #                 (RC(I,J),J=1,3),IRR(I),IRT(I)
      GO TO 159
  132 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
       WRITE(6,122)I,AID(J1),AID(J2),AID(J3),
     #                 (RC(I,J),J=1,3),IRR(I),IRT(I)
      GO TO 159
  133 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      J5=IRRR(I,5)
       WRITE(6,123)I,AID(J1),AID(J2),AID(J3),AID(J4),AID(J5),
     #                 (RC(I,J),J=1,3),IRR(I),IRT(I)
      GO TO 159
```

```
  134 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
       WRITE(6,124)I,AID(J1),AID(J2),AID(J3),
     #             (RC(I,J),J=1,3),IRR(I),IRT(I)
      GO TO 159
C-----------------------------------------------------PFS 6/6/83
  135 J1=IRRR(I,1)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
       WRITE(6,125)I,AID(J1),AID(J3),AID(J4),
     #             (RC(I,J),J=1,3),IRR(I),IRT(I)
      GO TO 159
C-----------------------------------------------------------------
  136 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
       WRITE(6,126)I,AID(J1),AID(J2),AID(J3),AID(J4),
     #             (RC(I,J),J=1,3),IRR(I),IRT(I)
      GO TO 159
  137 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
       WRITE(6,127)I,AID(J1),AID(J2),AID(J3),
     #             (RC(I,J),J=1,3),IRR(I),IRT(I)
      GO TO 159
  138 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      J5=IRRR(I,5)
       WRITE(6,128)I,AID(J1),AID(J2),AID(J3),AID(J4),AID(J5),
     #             (RC(I,J),J=1,3),IRR(I),IRT(I)
      GO TO 159
  139 J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
       WRITE(6,129)I,AID(J1),AID(J2),AID(J3),
     #             (RC(I,J),J=1,3),IRR(I),IRT(I)
      GO TO 159
C-----------------------------------------------------PFS 6/6/83
  140 J1=IRRR(I,1)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
       WRITE(6,130)I,AID(J1),AID(J3),AID(J4),
     #             (RC(I,J),J=1,3),IRR(I),IRT(I)
C-----------------------------------------------------------------
  159 CONTINUE
  160 WRITE(6,1968) MPSI, NS, NR, NT, FDL,DFDL, IRS,IMF,IPR,IINT,
```

```
     $ IXX, CPR, BBO, XIB, PB, CINT, CCHM
      WRITE(6,2047) NXC, PRNT
 2047 FORMAT(1H0,10X,'PRNT',8X,'NXC = ',I3/1H ,10X,1PE11.5/)
      WRITE(6,2048)
 2048 FORMAT(1H ,'PRNTXC (PRINT INTVLS AFTER THE 1ST) AND XCHANG (TIME
     $STATIONS AT WHICH CHANGE OVER TO PRNTXC)'/)
      WRITE(6,2049) (PRNTXC(IP),IP=1,NXC)
      WRITE(6,509)
      WRITE(6,2049) (XCHANG(IP),IP=1,NXC)
 2049 FORMAT(1H ,1P10E12.4)
C
C
      WRITE(6,*) PXIO
C
C
  161 CONTINUE
      IF(IET .EQ. 1) GO TO 162
      WRITE(6,7762)
 7762 FORMAT(1H1//////30X,'BEGIN NEXT ETA SET')
  162 CONTINUE
C
C
C
```

```
      WRITE(6,307) I,Y(I),PSI(I),BB(I),ATA(I),DINVD(I)
      WRITE(8,307) I,Y(I),PSI(I),BB(I),ATA(I),DINVD(I)
   74 CONTINUE
C
C
C* * * * *OUTPUT THE INITIAL CONDITIONS* * * * * * * * * * * * * * * * *
C
C
CJRB       CHANGE COMPOSITION PRINTOUT FROM 8 TO 9 PER LINE
      IRPT=(NS+8)/9
      WRITE(8,208) IRPT
      DO 564 KK=1,IRPT
      I1=1+(KK-1)*9
      I2=9+(KK-1)*9
      IF ( I2 .GT. NS ) I2 = NS
      WRITE(6,2201)
       WRITE(6,409)
       WRITE(8,108)(AID(J),J=I1,I2)
       WRITE(6,108)(AID(J),J=I1,I2)
C
C
C
C
        IONE = I1 + 5
        ITWO = I2 + 5
      DO 8111 I=1,MPSI
      DO 8011 II=I1,I2
      JJ = II - I1 + 1
      RPRMV(JJ) = ALPHA(II,I)*WTMIX
 8011 CONTINUE
C
C   RECALL THAT WORKING UNITS ALPHA = MOLE FRACTION / MIXTURE MOLEC. WT. =
C   MOLAR DENSITY / MIXTURE MASS DENSITY.
C
C   INPUT/OUTPUT UNITS ALPHA = MOLE FRACTION.
C
      JJ = I2 - I1 + 1
        WRITE(8,208)I,Y(I),(RPRMV(J),J=1,JJ)
       WRITE(6,208)I,Y(I),(RPRMV(J),J=1,JJ)
C
C
C
C
8111  CONTINUE
  564 CONTINUE
  163 CONTINUE
      IF(IIN .EQ. 0) GO TO 164
C
C
C
```

```
C   GEOMETRIC INPUTS
C
C
C
        WRITE(6,201) X ,(TITLE(I),I=1,18),IPAGE
        WRITE(6,222) NSTEP
        WRITE(6,102)
C
       WRITE(8,104) IET, ETAT, T, DENS, XI0, RATEIN, Z0,  RO
       WRITE(6,104) IET, ETAT, T, DENS, XI0, RATEIN, Z0,  RO
       WRITE(6,107)
        WRITE(6,509)
       WRITE(8,107)
        WRITE(8,208) MPSI
       DO 83 I=1,MPSI
       WRITE(6,307) I,Y(I),PSI(I),R(I),Z(I),H1(I),H2(I),R1(I),R2(I)
     $,Z1(I),Z2(I),DPDY(I)
       WRITE(8,307) I,Y(I),PSI(I),R(I),Z(I),H1(I),H2(I),R1(I),R2(I)
     $,Z1(I),Z2(I),DPDY(I)
   83 CONTINUE
C
       WRITE(6,510)
       WRITE(6,117)
       WRITE(6,509)
       WRITE(8,117)
       DO 84 I = 1,MPSI
       WRITE(6,307) I,Y(I),PSI(I),BB(I),ATA(I),DINVD(I)
       WRITE(8,307) I,Y(I),PSI(I),BB(I),ATA(I),DINVD(I)
   84 CONTINUE
  164 CONTINUE
C
C
C
C* * * * * * *OUTPUT THE YIELDS* * * * * * * * * * * * * * * * * * * * *
C
C
CJRB       CHANGE COMPOSITION PRINTOUT FROM 8 TO 9 PER LINE
       IRPT=(NS+8)/9
       WRITE(8,208) IRPT
       DO 4564 KK=1,IRPT
       I1=1+(KK-1)*9
       I2=9+(KK-1)*9
       IF ( I2 .GT. NS ) I2 = NS
       WRITE(6,2202)
        WRITE(6,410)
        WRITE(8,108)(AID(J),J=I1,I2)
        WRITE(6,108)(AID(J),J=I1,I2)
C
C
C
```

```
C
        IONE = I1 + 5
        ITWO = I2 + 5
      DO 48111 I=1,MPSI
      DO 48011 II=I1,I2
      JJ = II - I1 + 1
      RPRMV(JJ) = YI(II,I)
48011 CONTINUE
      JJ = I2 - I1 + 1
        WRITE(8,208)I,Y(I),(RPRMV(J),J=1,JJ)
        WRITE(6,208)I,Y(I),(RPRMV(J),J=1,JJ)
C
C
C
C
48111  CONTINUE
 4564  CONTINUE
C
C
  120 FORMAT(1H0,19X,26HREACTIONS BEING CONSIDERED,6X,15HKR=A*EXP(B/RT)/
     1,4HT**N,8X,1HA,8X,1HN,8X,1HB,4X,
     2 30HREACTION TYPE  RATE COEF. TYPE /)
  121 FORMAT(I9,9X,A4,2H+ ,A4,8X,2H= ,A4,2H+ ,A4,18X,
     #E10.4,2X,F4.1,1X,F10.1,11X,I2,15X,I1)
  122 FORMAT(I9,9X,A4,2H+ ,A4,3H+ M,5X,2H= ,A4,3H+ M,23X,
     #E10.4,2X,F4.1,1X,F10.1,11X,I2,15X,I1)
  123 FORMAT(I9,9X,A4,2H+ ,A4,8X,2H= ,A4,2H+ ,A4,2H+ ,A4,9X,
     #E10.4,2X,F4.1,1X,F10.1,11X,I2,15X,I1)
  124 FORMAT(I9,9X,A4,2H+ ,A4,8X,2H= ,A4,25X,
     #E10.4,2X,F4.1,1X,F10.1,11X,I2,15X,I1)
  125 FORMAT(I9,9X,A4,3H+ M,13X,2H= ,A4,2H+ ,A4,3H+ M,14X,
     #E10.4,2X,F4.1,1X,F10.1,11X,I2,15X,I1)
  126 FORMAT(I9,9X,A4,2H+ ,A4,8X,3H=> ,A4,2H+ ,A4,17X,
     #E10.4,2X,F4.1,1X,F10.1,11X,I2,15X,I1)
  127 FORMAT(I9,9X,A4,2H+ ,A4,3H+ M,5X,3H=> ,A4,3H+ M,22X,
     #E10.4,2X,F4.1,1X,F10.1,11X,I2,15X,I1)
  128 FORMAT(I9,9X,A4,2H+ ,A4,8X,3H=> ,A4,2H+ ,A4,2H+ ,A4,9X,
     #E10.4,2X,F4.1,1X,F10.1,11X,I2,15X,I1)
  129 FORMAT(I9,9X,A4,2H+ ,A4,8X,3H=> ,A4,25X,
     #E10.4,2X,F4.1,1X,F10.1,11X,I2,15X,I1)
  130 FORMAT(I9,9X,A4,3H+ M,13X,3H=> ,A4,2H+ ,A4,3H+ M,14X,
     #E10.4,2X,F4.1,1X,F10.1,11X,I2,15X,I1)
C-----------------------------------------------------------------------
C
C       FORMAT FOR REACTION 8 AS GIVEN FAILED TO INCLUDE THE 5TH SPECIES
C       CORRECTED 12/23/82 PFS.  ALSO = REPLACED BY => FOR RXNS 6-10.
C
C-----------------------------------------------------------------------
 1901 FORMAT(1H1///////20X,
     $          'ADAPTATION OF THE BOAT CODE TO TIME DEPENDENT DIFFUSION
```

```
      $ KINETICS FOLLOWING ELECTRON'/20X'BOMBARDMENT OF WATER VAPOR'///,
      $1H ,19X,'PAUL F. SCHIPPNICK & ALEX E. S. GREEN '
      $/1H ,19X,'UNIVERSITY OF FLORIDA'//1H ,30X,'1983'///)
 1902 FORMAT(1H0,18A4//)
 1916  FORMAT(1H0,48X,5X,6HCENTER,4X,4X,5X,4HEDGE,6X/)
 1917 FORMAT(23X,13HMOLE FRACTION,3X,A4,5X,  E15.7,4X,  E15.7)
 1908 FORMAT(1H0,10X,'X INITIAL (SEC) = ',E15.7,5X,'X FINAL (SEC) = ',
      $E15.7//)
 1968 FORMAT(1H0,10X,'MPSI  ',4X,'  NS  ',4X,'  NR  ',4X,'  NT  ',4X,
      $'  FDL '10X' DFDL '10X'IRS'4X'IMF'4X'IPR'4X'I1NT'3X'IXX'
      $/1H ,10X,I3,9X,
      $ 12,7X,I3,6X,I4,6X,1PE10.4,4X,E10.4,9X,5(I1,6X)//1H ,10X,
      $'CPR',9X,'BB0',9X,'XIB',9X,'PB',10X,'CINT',8X,'CCHM'/
      $1H ,8X,1P10E12.4)
C
C
C  FORMATS FOR SPATIAL COORDINATE INFORMATION, INITIAL CONDITIONS AND
C  YIELD  OUTPUT
C
  102 FORMAT(1H0,3X,'ETA PT',8X,'ETA',11X,'TEMP (K)',6X
      $,'DENS (#/CM3)     X10',8X,'RATE (#/SEC)  ',2X,'Z0 (CM)',7X,
      $ 'DENS (GM/CM3)')
  104 FORMAT(4X,I2,10X,1P8E14.6)
  107 FORMAT(5H0 PT , 7HXI (CM),4X, 8HXI PRIME,3X,6HR (CM),5X,
      1 6HZ (CM),5X, 2HH1,9X, 2HH2,9X, 2HR1,9X, 2HR2,9X, 2HZ1,9X,
      2 2HZ2,9X, 4HDPDY)
  117 FORMAT(5H0 PT , 7HXI (CM),4X, 8HXI PRIME,3X,6HB (XI),5X,
      $1HETA-LOCAL  ,5HDINVD)
  108 FORMAT(4H0 PT,3X,6HXI(CM),2X,9(3X,A4,4X))
  201 FORMAT(1H1,//3H X=  E15.7,6H SEC  ,8X,18A4,8X,4HPAGEI4)
  222 FORMAT(1H ,'NSTEP = ',I5)
 2201 FORMAT(1H1,'*******INITIAL CONDITIONS****',100(1H*)/)
 2202 FORMAT(1H1,'*******YIELDS***************',100(1H*)/)
  208 FORMAT(1H ,I3,2X,1PE11.4,  9E11.4)
  307 FORMAT(I4, 11(1PE11.4))
  409 FORMAT(1H0,44X,14HMOLE FRACTIONS)
  410 FORMAT(1H0,44X,14HMOLES/CC/SEC  )
  509 FORMAT(1H0)
  510 FORMAT(1H0///)
      RETURN
      END
-----------------------------
          A.SADK
-----------------------------
C
C
      DIMENSION XID(25)
C
C-----------------------------------------------------------------------
CPFS LATE FEBRUARY 1983  COMPACTION CORRECTION PER REACTIONS 5 AND 10
```

```
C
      LOGICAL L510
C-----------------------------------------------------------------------
C
C
C ****  THE FOLLOWING VARIABLES APPEAR IN COMMON AND ARE
C       INITIALIZED HERE
      MPSIX   = 101
      NSX     = 25
      NRX     = 80
      LUNIN = 2
C
      DATA AH20 /4HH20 /
C ****  END OF INITIALIZATION
C
C
C         FORMATS
  100 FORMAT(16I5)
  101 FORMAT (A4,1X,2E10.0)
  444 FORMAT (A4,3X,A4,10X,A4,3X,A4,3X,A4,9X,I2,I1,E8.2,F4.1,F9.1)
  555 FORMAT(20A4)
 1000 FORMAT(8E10.5)
 1050 FORMAT(5X,A4,1X,7E10.3)
 2000 FORMAT(5D15.7)
C
C
 1001 FORMAT(I1)
C
C
C
C*****************************************************************
      READ(2,333) (TITLE(I),I=1,18)
  333 FORMAT(18A4)
C
      READ(LUNIN,100)MPSI,NS,NR,IOUT1,IOUT2,IOUT3,IOUT4,IOUT5,IOUT6
C
      IF(MPSI .LE. 3) MPSI = 1
      NPSI = MPSI - 1
      IF(NPSI .LE. 0) NPSI = 1
C
C
      LPSI = MPSI + 1
C  NEVER USED, SINCE THE EDGE POINT IS EXTRAPOLATED, RATHER THAN
C  PROPAGATED ON THE BASIS OF EXTRAPOLATED DERIVATIVES
C
C*******************************************************************
C
C  INITIAL CONDITIONS FROM RESTART FILE IF IRS = 1, NORMAL IF IRS = 0
C
C  MOLE FRACTIONS ONLY IF IMF = 0;  MOLE FRACS. AND CONCENTRATIONS IF IMF .= 1
```

```
C
C   DISCRETE BLOCK PRINT INTERVAL IF IPR = 0;  PROPORTIONAL TO X IF IPR = 1
C   PROPORTIONALITY CONSTANT = CPR
C
C   REDISTRIBUTE GRID IF IINT = 1 --  FIXED IF IINT = 0
C
C   START UP WITH CHEMISTRY FRIENDLY TIME STEPS (DX = CHEM(X)) IF IXX = 1
C
C   WRITE OUT REACTION RATES IF IREAC = 1 ( .GE. 1)
C
      IRS = IOUT1
      IMF = IOUT2
      IPR = IOUT3
      IINT = IOUT4
      IXX = IOUT5
      IREAC = IOUT6
C
C.....................................................................
C   READ IN CPR, XIO-INITIAL, CINT AND CCHM HERE
C
C   RE: XIO-INITIAL:
C   SEE BELOW. THAT MEANS XIO-INITIAL FOR REFERENCE CASE
C   ACTUAL CASE IS SCALED TO REDUCE FROM THIS CASE
C
      READ(LUNIN,1000) CPR, XIOIN, CINT, CCHM
C
C   CCHM IS USED ONLY IF IXX = IOUT5 =1     1.  IN THIS CASE CCHM = XCHK,
C   THE TIME (SEC) AT WHICH THE CHEMISTRY TIME STEP PLATEAUS.
C.....................................................................
C
      CALL SFVFL (0.0, ALPHA, NSX * LPSI)
C.....................................................................
      READ(LUNIN,1000) XINIT,XMAX,PRNT,FDL,DXMIN
      READ(LUNIN,100) NXC
      READ(LUNIN,1000) (XCHANG(I),PRNTXC(I), I=1,NXC)
C
      IXC = 1
C   IXC IS A SWITCH  WHICH IS INITIALIZED HERE
C
C
C
      DFDL=1.
C.....................................................
C
C
      READ(LUNIN,1000) E0, T, DENS, RATEIN, Z0
C
C-  -  -  -
```

```
C   PREP.    CARE SHOULD BE TAKEN TO READ IN THE  S A M E VALUE.  Z0 IS
C   READ IN IN PREP AS GM(1 THROUGH 5).  THESE FIVE VALUES SHOULD ALL BE
C    IDENTICAL
C
C
      Z0 = Z0*6.E15/DENS
C-  - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C   SINCE WATER IS THE PREDOMINANT SPECIES WE CAN RIGHT AWAY CALCULATE
C   A CONSTANT INITIAL MASS DENSITY
C
C
      WTMIX = 18.020
      RO = WTMIX/6.0225E23*DENS
C   CGS UNITS
C
C   PRESSURE IN ATMOSPHERES:
      P = DENS*82.05/5.0225E23*T
C
C.....................................................................
C
      DXMIN=AMAX1(DXMIN,1.E-23)
C   PROTECT AGAINST PUTTING IN ZERO.  THIS ASSUMES THAT A DX BELOW 1.E-9
C   IS NOT WANTED
C.....................................................................
C
C
C   READ IN CENTRAL VALUE OF B AND TWO FALL-OFF PARAMETERS, AND CONSTANT
C   OUTER (EDGE) VALUE OF XI, XIEDGE
C
      READ(LUNIN,1000) BB0, XIB, PB, XIEDGE
C
C   XIEDGE SHOULD = ABOUT 35 TO 37 DIVIDED BY B23D
C   B23D = DOMINANT FALLOFF PARAMETER OF THE YIELDS
C   FOR YIELDS CALCULATED VIA PREP, B23D IS CALCULATED AS BT(2)*RO
C   I.E. IN TERMS OF THE ORIG BT: BT IS OVERWRITTEN BY EXACTLY THIS EXPRESSION
C
C
C.....................................................................
C   READ IN PARAMETERS CONTROLLING TIME DEPENDENCE OF XIO  (PXIO)
C   READ IN ANY OTHER PARAMETERS.  HERE IS SPACE FOR THEM
C
      READ(LUNIN,1000) (PXIO  (I), I = 1,8)
      READ(LUNIN,1000) (PXX1  (I), I = 1,8)
      READ(LUNIN,1000) (PXX2  (I), I = 1,8)
      READ(LUNIN,1000) (PXX3  (I), I = 1,8)
C
      B23D = PXIO(8)
      XIOIN = XIOIN*.242/B23D
C  REDUCE TO REFERENCE CASE: E0 = 1000 EV, N = 6*10**15 #/CC
```

```
C
C   OVERWRITE XIEDGE TO STANDARDIZE
C
      XIEDGE = 36./B23D
C
C
C*****************************************************************
      READ(LUNIN,100) NET
      READ(LUNIN,1333) (ETA(I), I = 1, NET)
 1333 FORMAT(8F10.7)
C   THIS IS TO TAKE ADVANTAGE OF THE RANGE OF ETA: -1 .LE. ETA .LE. 1
C   IN THIS WAY WE OVERCOME THE LIMITATIONS ON NUMBER OF DIGITS AFTER
C   THE DECIMAL SHOULD E-FORMAT HAVE BEEN USED. LIMIT 5 FOR POSITIVE
C   AND 4 FOR NEGATIVE ETA, IN WHICH CASE IF F-FORMAT OVERRIDE IS IMPLE-
C   MENTED. IT TURNS OUT (NASTY ) THAT THE E-FORMAT DECIMAL SPECIFICATION
C   CONTINUES TO HOLD, RESULTING IN NASTY ( ) ROUNDING OFF  (NOT TRUNCA-
C   TION) (EITHER ONE WE SHOULD LIKE?)
C
C*****************************************************************
C
C
C
      READ(LUNIN,555) (AID(J), J=1,NS)
      READ(LUNIN,1000) (WTMOLE(J), J=1,NS)
      READ(LUNIN,2000) (AL(J), J=1,NS)
      READ(LUNIN,2000) (BL(J), J=1,NS)
      READ(LUNIN,2000) (CL(J), J=1,NS)
C
      DO 1800 J=1,NS
 1800 READ(LUNIN,2000) (CON(I,J), I=1,14)
C
      IF(NR.EQ.0) GO TO 1875
C
      DO 1892 I=1,NR
      READ(LUNIN,444) (ZID(J),J=1,5), IRR(I), IRT(I), (RC(I,K),K=1,3)
      L510 = IRR(I).EQ.5.OR.IRR(I).EQ.10
      M = 1
      DO 1893 J=1,5
      IRRR(I,J) = 0
 1891 DO 1894 L=1,NS
      IF(ZID(M)-AID(L)) 1894,1895,1894
 1894 CONTINUE
      M = M + 1
      IF( M .LE. 5 ) GO TO 1891
      GO TO 1896
 1895 IRRR(I,J) = L
      M = M + 1
 1893 CONTINUE
 1896 IF(.NOT.L510) GO TO 1892
      IRRR(I,4) = IRRR(I,3)
```

```
      IRRR(I,3) = IRRR(I,2)
      IRRR(I,2) = 0
 1892 CONTINUE
C
CPFS2/4/83 NOTE COMPACTION PROCEDURE IF ZID(M) = 'M    ' OR '    '.
C          GO TO 1891 SHORT CIRCUITS CODA OF DO LOOP (STA. NO 1893), SO
C          THE J COUNTER DOES NOT GET UPPED.
C
CPFS 4/23/83 PUT LATE FEBRUARY'S WORK BACK IN HERE TO CORRECT FOR COMPACTION
C            OF REACTION TYPES 5 AND 10  --  GOT ZAPPED WHEN I RELEASED THE
C            METHANE FILE, FORGETTING THAT I HAD NOT TRANSFERRED THIS JUICY
C            BIT OF INFO TO THE 'H2' FILE.
C
C
C
 1875 CONTINUE
C
C
C
C-----------------------------------------------------------------------
C  READ IN AND REGURGITATE DIFFUSION COEFFICIENTS (AT T = 300 K)


      WRITE(6,10510)
10510 FORMAT(1H0,'AID ',3X,'XID ',4X,'DFCOEF'/)
      DO 1024 I=1,NS
      READ(5,1050) XID(I), DFCOEF(I)
      DFCOSV = DFCOEF(I)
      DFCOEF(I) = DFCOSV*(T/300.)**1.67/P
 1023 CONTINUE
      WRITE(6,10511) AID(I), XID(I), DFCOSV, DFCOEF(I)
 1024 CONTINUE
10511 FORMAT(1H ,A4,3X,A4,4X,2(E11.4,2X))
C-----------------------------------------------------------------------
      J    = 1
      JH20 = 0
      DO 1025 I = 1, NS
      IF(AID(I) .EQ. AH20) JH20 = I
      IF (DFCOEF(I) .GE. DFCOEF(J)) J = I
 1025 CONTINUE
      DFCOMX = DFCOEF(J)
C
C-----------------------------------------------------------------------
  600 FORMAT(20A4)
      RETURN
      END
-----------------------------
          A.SBDKRS
-----------------------------
C
```

```
      DIMENSION SEND(10)
      REAL*8 XIARR(2001), RHOARR(2001), ZZARR(2001)
      COMMON /NRB/ SEND, INR
      COMMON /STORE/ XIARR, RHOARR, ZZARR
C
C*************************************************************
C
C  INITIALIZE X, XIO, AND THE GRID HERE
C  (INITIALIZE OR RE-INITIALIZE)
C
      X = XINIT
      XIO    = XIOIN
      XIOSAV = XIOIN
      XIOINT = XIOIN
C
      NSTEP = 0
C*************************************************************
C
C  ALERT:  Y(I) = XI    PSI(I) = XI PRIME =  LN (XI/XIO + 1)
C  NOTE:  PSI(I) ARE EQUALLY SPACED
C
      DELPSI = ALOG( XIEDGE/XIO + 1. )/FLOAT(NPSI)
C
C     INITIALIZE THE PSI/Y GRID, AND THE ARRAYS BB, DPDY, AND DINVD.
      DO 7 I=1,LPSI
C
      PSI(I) = DELPSI*FLOAT(I - 1)
      Y(I) = XIO*(EXP(PSI(I)) - 1.)
      BB(I) = 1. + (BB0 - 1.)/(1.+ (Y(I)/XIB)**PB)
C
C  DPDY = D(PSI)/DY, I.E. = D(XI PRIME)/DXI
C  DINVD = D/DPSI (DPSI/DY)
C        = (1/XIO)*D/DPSI (EXP(-PSI)) = - (1/XIO)*EXP(-PSI) = -DPDY
C
      DPDY(I) = 1./(Y(I) + XIO)
      DINVD(I) = -DPDY(I)
    7 CONTINUE
C*************************************************************
      SEND(1) = BB0
      SEND(2) = XIB
      SEND(3) = PB
      SEND(4) = XIO
      SEND(5) = XIEDGE
C
C
C
C     CALCULATE GIBBS FREE ENERGY FOR ASSORTED SPECIES
C     CONSTANT TEMPERATURE REGIME - ONLY INITIAL CALCULATION NEEDED
C
      CALL BOATGX
```

```
C
C
C
C     INITIALIZE PRINT LOOP CONTROL PARAMETERS
C
      IFINIS = 0
      PCNT = 0.
C
C
C     INITIALIZE THE ON-OFF SWITCH FOR BOATIN
C
      IIN = 0
C
C
C
C     INITIALIZE THE CONCENTRATIONS FOR ALL SPECIES
C
      CALL SFVFL(0., ALPHA, 2525)
C
C.......................................................RESTART OR REGULAR INPUT?
      IF(IRS .EQ. 1) GO TO 5500
      CALL BOATIC
      GO TO 5501
 5500 CONTINUE
      CALL LOCORS
 5501 CONTINUE
C
C
C
      IF(IDIAG.EQ.0) GO TO 8451
      DO 849 I = 1, MPSI
      WRITE(6,9449) (ALPHA(J,I),J=1,NS)
  849 CONTINUE
      WRITE(6,8450)
 8450 FORMAT(1H ,'BEGIN OF SB'///)
 8451 CONTINUE
C
C
C
C     CONVERT MOLE FRACTIONS TO WORKING UNITS
C
      DO 1900 I=1,MPSI
      DO 1900 J=1,NS
      ALPHA(J,I) = ALPHA(J,I)/WTMIX
 1900 CONTINUE
C
C
C   WTMIX = MIXTURE MOLECULAR WEIGHT (M).  RO = M*N.  N = MIXTURE
C   M O L A R  NUMBER DENSITY.  RO IS MASS DENSITY.
C
```

```
C   ALPHA INPUT-OUTPUT IS MOLE FRACTION.  WORKING UNITS, IT IS MOLE FRACTION
C   DIVIDED BY MIXTURE MOLEC. WT.  MULTIPLYING THEN BY RO, WE GET SPECIES
C   M O L A R NUMBER DENSITY.
C
C*****************************************************************
      IF(IDIAG.EQ.0) GO TO 9451
      DO 949 I = 1, MPSI
      WRITE(6,9449) (ALPHA(J,I),J=1,NS)
  949 CONTINUE
 9449 FORMAT(1H ,1P8E14.5)
      WRITE(6,9450)
 9450 FORMAT(1H ,'END OF SB'///)
 9451 CONTINUE
C*****************************************************************
C
C
C
C-----------------
      INR = 0
C-----------------
C
C   IF MPSI = 1, INR IS IRRELEVANT
      R(1) = 0.
      Z(1) = 0.
C   EVEN THESE HARDLY MATTER
      IF(MPSI .EQ. 1) GO TO 1155
C
C-----------------
      CALL BOATNR( Y, ETAT, BB, Z0, LPSI, R, Z, R1, R2, Z1, Z2, H1, H2,
     $ ATA)
C-----------------
C
 1155 CONTINUE
C
C-----------------
      INR = 1
C-----------------
C
C
C2222 FORMAT(1H0,'SB-----SB-----SB-----SB-----SB'/)
C2223 FORMAT(1H0)
C2224 FORMAT(1H ,1P10E12.5)
C2225 FORMAT(1H ,1P10D12.5)
C     WRITE(6,2222)
C     WRITE(6,2223)
C     WRITE(6,2224) (R(I),I=1,LPSI)
C     WRITE(6,2224) (Z(I),I=1,LPSI)
C     WRITE(6,2224) (ATA(I),I=1,LPSI)
C     WRITE(6,2223)
C     WRITE(6,2225) (XIARR(I),I=1,2001)
```

```
C       WRITE(6,2225) (RHOARR(I),I=1,2001)
C       WRITE(6,2225) (ZZARR(I),I=1,2001)
C       WRITE(6,2222)
C
C
C
C-----------------------------------------------------------
        IF(MPSI .EQ. 1) GO TO 1156
        DO 10 I = 1, LPSI
C     COORDINATE TRANSFORMATION : XI --> XI PRIME
C
C    XI PRIME = LN ( XI/XI0 + 1 )
C
        R1P(I) = R1(I)/DPDY(I)
        Z1P(I) = Z1(I)/DPDY(I)
        H1P(I) = H1(I)/DPDY(I)
C
        A(I) = H2(I)*R(I)/H1P(I)
        TRIP(I) = H1P(I)*H2(I)*R(I)
C
C   H1 VARIES FROM 1 AT ETA = 0 TO 8 AT ABS(ETA) = 1
   10 CONTINUE
 1156 CONTINUE
C-----------------------------------------------------------
C
C       COMPUTE THE YIELDS
C
C
        CALL BOATYI
C
C   OUTPUT HEADER (IET = 1) OR MINIHEADER (IET > 1), GEOMETRY,
C   INITIAL CONDITIONS AND YIELDS
C   IN SUBSEQUENT CALLS OF BOATIN FROM BOATM2 ONLY OUTPUT GEOMETRY
C                          AND YIELDS
C
        CALL BOATIN
C
C       SWITCH  IIN TO ON.  STAYS THERE FOR REST OF THIS ETA LOOP
C
        IIN = 1
C
        RETURN
        END
-----------------------------
          B.OTDKRS
-----------------------------
C
        DIMENSION   RPRMV(10), JOJO(25)
C
C-------------------------------------------
```

```
C
      DO 1112 I = 1, 25
 1112 JOJO(I) = I
C
C-----------------------------------------
C
C
CJRB       CHANGE COMPOSITION PRINTOUT FROM 8 TO 9 PER LINE
      IRPT=(NS+8)/9
      IF(MPSI .GT. 1) WRITE(8,208) IRPT
C
C  OUTPUT THE MOLE FRACTIONS
C  IF IMF = 1 SKIP THE PRINTOUTS BUT ASSIGN ALF(J,I)
      IF(IMF .EQ. 1) GO TO 463
      DO 464 KK=1,IRPT
      I1=1+(KK-1)*9
      I2=9+(KK-1)*9
      IF ( I2 .GT. NS ) I2 = NS
       WRITE(6,202) X ,(TITLE(I),I=1,18),IPAGE,DX, NSTEP
C-----------------------------------------------------------------------
C 6/12/84 INSERT WRITE 8  READ READ READ READ READ READ READ READ READ READ
       WRITE(8,202) X ,(TITLE(I),I=1,18),IPAGE,DX, NSTEP
C-----------------------------------------------------------------------
       WRITE(6,409)
       IF(MPSI .GT. 1) WRITE(8,108)(AID(J),J=I1,I2)
       WRITE(6,108)(AID(J),J=I1,I2)
C
C
C
C
  463 CONTINUE
      DO 8111 I=1,MPSI
      DO 8011 II=I1,I2
      JJ = II - I1 + 1
      RPRMV(JJ) = ALPHA(II,I)*WTMIX
C
      ALF(II,I) = RPRMV(JJ)
C  FOR RESTART FILE - DISK D ATA SET
C
 8011 CONTINUE
      IF(IMF .EQ. 1) GO TO 8111
      JJ = I2 - I1 + 1
       WRITE(8,208)I,Y(I),(RPRMV(J),J=1,JJ)
       WRITE(6,208)I,Y(I),(RPRMV(J),J=1,JJ)
C
C
8111  CONTINUE
C
 2000 FORMAT(1H ,1P10E12.4)
C
```

```
  464 CONTINUE
  465 CONTINUE
C
C
C   OUTPUT THE MOLAR CONCENTRATIONS
C   IF IMF = 0 SKIP THIS
      IF(IMF .EQ. 0) GO TO 665
C
C
      DO 664 KK=1,IRPT
      I1=1+(KK-1)*9
      I2=9+(KK-1)*9
      IF ( I2 .GT. NS ) I2 = NS
       WRITE(6,202) X ,(TITLE(I),I=1,18),IPAGE,DX, NSTEP
C-----------------------------------------------------------------------
C 6/12/84 INSERT WRITE 8  READ READ READ READ READ READ READ READ READ READ READ
       WRITE(8,202) X ,(TITLE(I),I=1,18),IPAGE,DX, NSTEP
C-----------------------------------------------------------------------
       WRITE(6,509)
       IF(MPSI .GT. 1) WRITE(8,108)(AID(J),J=I1,I2)
       WRITE(6,108)(AID(J),J=I1,I2)
C
C
      DO 9111 I=1,MPSI
      DO 9011 II=I1,I2
      JJ = II - I1 + 1
      RPRMV(JJ) = RO*ALPHA(II,I)
 9011 CONTINUE
      JJ = I2 - I1 + 1
        WRITE(8,208)I,Y(I),(RPRMV(J),J=1,JJ)
       WRITE(6,208)I,Y(I),(RPRMV(J),J=1,JJ)
C
C
9111  CONTINUE
C
  664 CONTINUE
  665 CONTINUE
C
      RETURN
C
C
      ENTRY BOATO1
C
C   HERE WRITE OUT THE RESTART FILE (UNIT 9) AND COPY TO UNIT 6
C
      WRITE(6,2120)
 2120 FORMAT(1H1,'RESTART FILE FOR THIS VALUE OF ETA'//)
 2121 FORMAT(1H ,3X,I3,1P10E12.5)
 2122 FORMAT(1H ,3X,I3,1X,I7)
 2123 FORMAT(1H ,3X,I3,F10.7,1P9E12.5)
```

```
      WRITE(6,2122) MPSI, NSTEP
      WRITE(9,2122) MPSI, NSTEP
      WRITE(6,2123) IET, ETAT, X, XIO, BBO, XIB, PB, DENS, RATEIN, EO, T
      WRITE(9,2123) IET, ETAT, X, XIO, BBO, XIB, PB, DENS, RATEIN, EO, T
      DO 3210 I = 1, LPSI
      WRITE(6,2121) I, Y(I), PSI(I), ATA(I), H1(I), H2(I), BB(I),
     $                DPDY(I), DINVD(I), R(I), Z(I)
      WRITE(9,2121) I, Y(I), PSI(I), ATA(I), H1(I), H2(I), BB(I),
     $                DPDY(I), DINVD(I), R(I), Z(I)
 3210 CONTINUE
      WRITE(6,2119) (JOJO(J), J = 1, NS)
 2119 FORMAT(1H ,6X,10I12)
      DO 3211 I = 1, MPSI
      WRITE(6,2121) I, (ALF(J,I), J = 1, NS)
      WRITE(9,2121) I, (ALF(J,I), J = 1, NS)
 3211 CONTINUE
C
      RETURN
C
C
      ENTRY BOATO2
C
      IF(IREAC)567,567,75
   75 IRPT=(NR+9)/10
      N=0
      NNR=NR-1
C
      DO 565 KK=1,IRPT
      LL=0
      N=N+1
       WRITE(6,201) X ,(TITLE(I),I=1,18),IPAGE
   65 I1=1+(N-1)*5
      I2=5+(N-1)*5
      IZERO = 0
      IF ( I2. GT. NR )  IZERO = I2 - NR
      NNN1=I1
      NNN2=I1+1
      NNN3=I1+2
      NNN4=I1+3
      NNN5=I2
      WRITE(6,209)
       WRITE(6,431)NNN1,NNN2,NNN3,NNN4,NNN5
       WRITE(6,432)
      DO 631 I=1,MPSI
C
C
 63   NREC = (I-1)*NR + I1
       CALL SFVMV ( RPRM(NREC), RPRMV, 10 )
C
      IF ( IZERO .GT. 0 ) CALL SFVFL(0.,RPRMV(10-IZERO*2+1),IZERO*2)
```

```
C
C
 631  WRITE(6,433)I,Y(I),RPRMV,I
C
C
  566 IF(NNR/(5*N))565,565,64
   64 IF(LL)565,66,565
   66 N=N+1
      LL=1
      GO TO 65
  565 CONTINUE
  567 CONTINUE
  103 FORMAT(4X,  8E14.6)
  104 FORMAT(4X,I14,8E14.6)
  108 FORMAT(3H0PT,1X,7HXI (CM),3X,9(3X,A4,4X))
  201 FORMAT(1H0,//////3H X=  E15.7,6H SEC  ,8X,18A4,8X,4HPAGEI4)
  202 FORMAT(1H0,//////3H X=  E15.7,6H SEC  ,8X,18A4,8X,4HPAGEI4
     $ /1H0, 4H DX=  E15.7,6H SEC  ,3X,'NSTEP =',I7)
  208 FORMAT(I3,E12.4,  9(1PE11.4))
  209 FORMAT(1H ,//40X,28HREACTION RATES (MOLE/CC-SEC)//)
  307 FORMAT(I4, F8.4, 10(1PE12.5))
  409 FORMAT(1H0.44X,14HMOLE FRACTIONS)
  509 FORMAT(1H0.38X,'MOLAR CONCENTRATIONS (MOLE/CC)')
  431 FORMAT(1H0,2HPT,4X,3HXI  , 3X,5(8HREACTION,I3,11X),2HPT)
  432 FORMAT (9X,5(10X,2HRP,9X,2HRM))
  433 FORMAT(I3.1X,  11E11.4,I4)
      RETURN
      END
-----------------------------
        YI.1000S
COMMENT:  PLUME INTEGRALS FOR THE VARIOUS STATES.  OUTPUT OF YH2O.
-----------------------------
  1000.00     1   0.5878806E+01  0.1470071E+03  0.4265398E+01  0.5178476E-01
  1000.00     2   0.1201526E+02  0.2591135E+03  0.1333746E+00  0.5276019E-01
  1000.00     3   0.1174391E+01  0.2318906E+02  0.3242161E-04  0.5276021E-02
  1000.00     4   0.3708142E-01  0.5370228E+00  0.0            0.1908433E-07
  1000.00     5   0.5757571E-01  0.1945013E+00  0.0            0.1364458E-06
  1000.00     6   0.2076695E+01  0.2985768E+01  0.0            0.1743269E-01
  1000.00     7   0.2204500E+01  0.1429856E+01  0.0            0.2152525E-01
  1000.00     8   0.5512657E+01  0.8199461E+00  0.0            0.8160448E-01
  1000.00     9   0.2825458E+01  0.5147757E-10  0.0            0.6138599E-01
  1000.00    10   0.4520634E+00  0.5954804E-11  0.0            0.7343885E-02
  1000.00    11   0.1674332E+01  0.4089003E+01  0.0            0.1073090E-01
  1000.00     1   0.5671554E+00  0.2998071E+00  0.0            0.6427195E-02
  1000.00     2   0.5548379E+00  0.2859349E+00  0.0            0.6328363E-02
  1000.00     3   0.1026181E+01  0.3573501E+00  0.0            0.1276368E-01
  1000.00     4   0.1026181E+01  0.3573501E+00  0.0            0.1276368E-01
  1000.00     1   0.1066289E+02  0.1845004E+01  0.0            0.2199578E+00
  1000.00     2   0.8268395E+01  0.7435259E+00  0.0            0.1789819E+00
  1000.00     3   0.9250270E+01  0.4508365E+00  0.0            0.1845878E+00
```

```
  1000.00     4   0.2529460E+01  0.2053532E-11  0.0                0.7070249E-01
   0.1500E07   0.1350E07   0.1350E07   0.2500E07   0.1300E07
       .9850       .9700       .9700       .9850       .9700
      8.600       8.600       8.600       8.600       8.600
 5  0  8 12 13 14 15
 3  1  7 18 19
1.0  .100 .25
 7  0  8 12 13 14 15 16 17
 0
 6  1  6  9 10 11 18 19
1.    1.    1.    1.    .07  .75
 5  1  6  9 10 11 18
1.    1.    1.    1.    .830
 1  0  7
 0
 0
 0
 0
 0
 1  1 18
.830
 2  1 18 19
.070 .75
-----------------------------
        DDD.DFNE
COMMENT:  DIFFUSION COEFFICIENTS
-----------------------------
     H          1.2916
     H2         0.8644
     H2O        0.2502
     HO2        0.2339
     H2O2       0.2327
     O          0.3754
     OH         0.3695
     O2         0.2305
-----------------------------
******************************
-----------------------------
```

APPENDIX B

```
-----------------------------
            ADIABAT
-----------------------------
@@ETA JOB (2003,5006,200,20),'PAUL SCHIPPNICK',REGION=950K,CLASS=T
@*PASSWORD
@*ROUTE PRINT LOCAL
@@ EXEC FORTXCG,LPARM='SIZE=950K'
```

```
C-----------------------------------------------------------------------
C
C
C-----------------------------------------------------------------------
C
      DIMENSION ZZ(10001), RHO(10001), XIARR(10001), ETARR(50)
      DIMENSION ATARR(10001), BARR(10001)
C
C
C
C
C   IF IZ = 1 WRITE OUT Z ARRAY
C   IF IW2 = 1 WRITE OUT RHO ARRAY FOR ETA CONTOURS
C          AND ETA AND BB
C
      IZ = 1
      IW2 = 1
C
      ZMIN = 0.
C
C   CYCLE THRU PLOTS
C
      READ(5,*) NPLOTS
      DO 7500 KYKLOS = 1,NPLOTS
      READ(5,*) NC, XIMAX, BB, NZ
C
C
      READ(5,100) (ETARR(I),I=1,NC)
  100 FORMAT(8E10.3)
C
C
C
      WRITE(6,*) NC, XIMAX, BB, NZ
      WRITE(6,102)
  102 FORMAT(1H0)
      WRITE(6,101) (ETARR(I),I=1,NC)
  101 FORMAT(1H ,1P10E12.5)
C
      WRITE(6,102)
C
C
C
C
C*****************************************************************************
      DO 10015 I = 1,NC
      ETA = ETARR(I)
      ETAP = ETA/SQRT(1.E0 - ETA*ETA)
C
C
C   CRUDE ESTIMATE OF ZMAX (UPPER BOUND)
```

:

```
C
C   ZMAX = BB*XIMAX*ETA
C
      ZMAX = BB*XIMAX*ETA
C
C
      DZ = ZMAX - ZMIN
      ZINTVL = DZ/(NZ - 1)
C-----------------------------------------
      ZC = 3.*ZINTVL
C-----------------------------------------
      DO 10 L = 1,NZ
   10 ZZ(L) = ZMIN + ZINTVL*(L-1)
C
      IF(IZ .EQ. 1) WRITE(6,101) (ZZ(M),M=1,NZ)
C
C
C
      M = 0
      K = NZ + 1
        DO 10014 J = 1,NZ
        Z = ZZ(J)
C
C
      IF(M .EQ. 1) GO TO 3001
      IF (Z .GT. ZC) M = 1
      IF(Z .GT. ZC) K = J
 3001 CONTINUE
C   INITIAL Z POINTS (0 .LE. Z .LE. ZC+ZINTVL) APPROXIMATE ATA BY ETA:
C
      IF(J .GT. K) GO TO 93
      ATARR(J) = ETA
      BARR(J) = BB
      B = BB
C
      RHO(J) = Z**(B*B)/ETAP
      R = RHO(J)
      XIARR(J) = SQRT(R*R + Z*Z/B/B)
C
      IF(M .EQ. 0) GO TO 10013
   93 CONTINUE
C
C
C   ABOVE LOGIC:  M=0 UNTIL Z .GT. ZC AT WHICH POINT IT BECOMES =1 AND
C   STAYS SO.  UP TO HERE WE WANT TO GO THRU THIS PRE-BLOCK ONLY. AT THIS
C   SWITCH-OVER POINT WE WANT TO GO THRU BOTH PRE-BLOCK AND FOLLOW-BLOCK.
C   AFTER THIS SWITCH-OVER POINT WE WANT TO GO ONLY THRU FOLLOW-BLOCK.
C
C   THIS IS EFFECTED BY ISOLATING THE SWITCH SO ONCE IT IS THROWN IT IS
C   NO LONGER IN THE FLOW AND MATING WITH IT THE K = J SET-SWITCH. SO THAT
```

```
C  NOW WE CAN TEST FOR J=K OR J .GT. K.
C
C*********************************************************************
C  FIND RHO BY EULER METHOD: SOLUTION OF FIRST ORDER NORMAL DE
C  UPDATE B BY ITERATIVE CONVERGENCE.
C
      RHO(J+1) = RHO(J)*(1. + B*B*ZINTVL/Z)
      R        = RHO(J+1)
      Z        =  ZZ(J+1)
C
      DO 77 ITER = 1, 99
      XIKES = SQRT(R*R + Z*Z/B/B)
      BSAV = B
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  APPROXIMATE SOLUTION TO STEADY STATE AXISYMMETRIC DIFFUSION:
C
      DATA DELO, DELP, XIBO, XIB1/ .59, .83, .63, 1.12 /
C
      DEL = DELO*(BB - 1.)**DELP
      XIB = XIBO + XIB1*(BB - 1.)
      B = 1. + DEL*EXP(-XI/XIB)
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
      REL = 1. - B/BSAV
      REL = ABS(REL)
C
C  B IS DESCENDING AS IT CONVERGES TO ITS HERE-VALUE FROM ITS INITIAL ESTIMATE
C  BECAUSE AS WE MOVE OUTWARD IN Z., THE INITIAL ESTIMATE, BEING THE PREVIOUS
C  VALUE OF B, IS HIGHER THAN THE NOW TO BE FOUND HERE-VALUE OF B.
C  HOW'S THAT FOR GERMAN WRITTEN WITH ENGLISH WORDS?
C
C  OF COURSE, THAT'S ASSUMING THAT B VARIES SO SLOWLY WRT Z RE: ZINTVL THAT
C  XIKES IS SATISFACTORILY ESTIMATED USING THE OLD VALUE OF B, I.E. IT IS
C  NOT UNSTABLY PERTURBED.
C
      IF(REL .LE. 1.E-7) GO TO 78
   77 CONTINUE
   78 CONTINUE
C
      BARR(J+1) = B
      ATAP = Z**(B*B)/R
      ATARR(J+1) = ATAP/SQRT(1. + ATAP*ATAP)
      XIARR(J+1) = SQRT(R*R + Z*Z/B/B)
C
10013 CONTINUE
10014 CONTINUE
C
C*********************************************************************
C
      IF(IW2 .EQ. 1) WRITE(6,101) (RHO(J),J=1,NZ)
      IF(IW2 .EQ. 1) WRITE(6,101) (ATARR(J),J=1,NZ)
```

```
      IF(IW2 .EQ. 1) WRITE(6,101) (XIARR(J),J=1,NZ)
      WRITE(6,102)
C
C-----------------------------------------------------------------------
C
C
10015 CONTINUE
C
 7500 CONTINUE
C
C
      STOP
      END
@@GO.SYSIN DD *
7.   7.   0.   14.
12  100.  2.0    1001
.0001      .001       .01        .05        .1         .3         .5         .7
.9         .99        .999       .9999
-----------------------------
*****************************
-----------------------------
```

```
-----------------------------
******************************
-----------------------------
              YH2OSUM
COMMENT:  WRITTEN BY DAN RIO (1983).  MINOR CHANGE HERE IN FORM OF
TWO DIMENSIONAL YIELD SPECTRA.  DISKFILE WRITTEN BY THIS PROGRAM IS
INPUT TO ALPHA.  THIS PROGRAM PROPERLY BELONGS UNDER THE HEADING OF
CHAPTER II, AND IS PUT HERE AS AN ADDENDUM.
-----------------------------
@@YH2OSUM JOB (2003,5006,60,5,10),SCHIPPNICK,CLASS=2,REGION=1000K
@*PASSWORD
@*ROUTE PRINT N1R0
@@ EXEC FORTXCG,LPARM='SIZE=3500K,MAP'
@*INCLUDE YIELD.AS  70003791,1
@*INCLUDE YIELD.B  70003791,1
@*INCLUDE UT.VM1D 20035006,12
@@GO.FT09F001 DD DSN=JF.B0035006.S1.YNEWSUM,UNIT=SYSDA,
@@ DISP=(NEW,CATLG),SPACE=(6160,(S,5),RLSE),
@@ DCB=(RECFM=FB,BLKSIZE=6160,LRECL=80)
@@*GO.FT09F001 DD DUMMY
@@GO.SYSIN DD *
1
111
 11  3  4  4
 1 2 3 4 5 6 7 8 91011
 1 2 3 4
 1 2 3 4
 1 1
   20.
   50.
   100.
   200.
   500.
   1000.
   3000.
  10000.
1 30000.
48
20.0      19.0      18.0      17.0      16.0      15.0      14.0      13.0
12.0      11.0      10.5      10.0      9.0       8.0       7.0       5.0
4.0       3.5       3.0       2.5       2.0       1.5       1.0       .90
.80       .70       .66       .64       .62       .60       .58       .56
.54       .52       .50       .48       .46       .44       .40       .36
.32       .28       .24       .20       .19975    .19925    .19875    .1985
1.116     1.043     .9691     .9109     .8527     .8045     .7563     .7230
.6897     .6683     .6550     .6283     .6334     .6411     .6497     .6521
.6361     .6186     .5908     .5495     .4936     .4462     .6605     .8918
1.320     2.522     3.376     3.849     4.279     4.579     4.669     4.544
4.262     3.913     3.570     3.274     1.340     1.435     1.627     1.804
1.935     1.990     1.955     1.837     1.836     1.835     1.833     1.831
```

```
(A1)V2                  0.198 0.198 0.0    1.00   5.193 .239   0.0000254
  1.347E-01   6.768E-02  2.750E-01
(A1)V1(B1)V3            0.460 0.460 0.0    1.00   6.09  .500   0.000850
  4.950E-02   1.300E-02  5.870E-01
(B1)V1(B1)V3            0.460 0.899 0.0    1.00   6.09  .500   0.000085
  4.950E-03   1.300E-02  5.870E-01
TRIPLET                 4.500 4.500 0.0    1.00   3.0   3.00   0.007000
TRIPLET                 12.50 9.810 0.0    1.00   1.0   3.00   0.018000
DIS. CONT.              7.400 7.400 0.0    1.00   3.0   0.75   0.063000
DIS. CONT.              9.670 9.670 0.0    1.00   3.0   0.80   0.138000
DIFFUSE BANDS           13.32 14.73 0.0    1.00   3.0   0.75   0.626000
H* LYMAN ALPHA          17.00 17.00 0.0    0.60   6.00  1.3    9.94500
H* BALMER ALPA          19.00 18.50 0.0    0.75   3.0   1.0    0.266000
OH* 3064A               10.00 9.500 0.0    0.45   0.65  .725   0.053750
SERIES A                9.9980 1.000 3.000 0.729 0.750 0.427 12.620
SERIES B                9.9980 1.000 3.000 0.700 0.750 0.438 12.620
SERIES C                11.060 1.000 3.000 0.050 0.750 1.850 12.620
SERIES D                11.060 1.000 3.000 0.050 0.750 1.850 12.620
1B1 H2O+                12.62   2.590   173.1   1.00   -5.58   0.00
                        11.4    0.0    -2.37   0.0     0.0
3A1 H2O+                14.75   2.115   176.4   1.00   -10.39  0.00
                        11.4    0.0    -2.37   0.0     0.0
1B2 OH+,H+,O+           18.51   2.069   116.2   1.00   -7.885  0.00
                        11.4    0.0    -2.37   0.0     0.0
2A1 H+,O+               32.40   .8842   241.0   1.00   -30.0   0.00
                        11.4    0.0    -2.37   0.0     0.0
-------------------------------
-------------------------------
          YIELD.AS
-------------------------------
C
      DIMENSION E(20)
      DIMENSION RALFA(4),RTHRI(4),RBETA(4),RO(4),RFF(4),RDELTA(4)
      DIMENSION RTHR(4)
      DIMENSION THRI(5),AKI(2,6),AJI(3,6),TDI(3,6),GAMAI(2,6)
      DIMENSION WF(23),WFA(23),FACI(23),ALFA(23),BEFA(23),CFA(23),
     #FFA(23),VIB1(23),VIB2(23),VIB3(23)
C
C
      DIMENSION GG1(30),GG2(30),GG3(30),GG4(30)
      DIMENSION GR1(4),GR2(4),GR3(4),GR4(4)
      DIMENSION GI1(10),GI2(10),GI3(10),GI4(10)
      DIMENSION TCSGEN(30,20),TCSRYD(4,20),TCSION(10,20)
      DIMENSION EIT(60),CSIE(60)
      DIMENSION Y(20,30,4,3),ER(20,30,4,3)
C
      DIMENSION ITYPE(3),ISTATG(30),ISTATR(4),ISTATI(10)
C
      COMMON/CONST/  QO
      COMMON/PARAG/ WF,WFA,FACI.ALFA.BEFA,CFA,FFA.VIB1,VIB2,VIB3
```

```
      #,ISWV,KV
       COMMON/PARAR/ RTHRI,RALFA,RBETA,RO,RDELTA,RFF,RTHR
       COMMON/PARAI/ THRI,AKI,AJI,GAMAI,TOI
C
       COMMON/FUNTCS/ EIT,CSIE,TCSG,TCSR,TCSI,IEILM1
       COMMON/FUNSW/ K,N,J,EK
C
C
C CONSTANTS
        Q0=651.3
C
C ***************************************************************
C *                INPUT GENERAL SWITCHES,ETC.                  *
C *                                                             *
C *    INPUT ENERGY VECTOR OPTION :INEVEC=0 ->FULL VECTOR       *
C *                                =1 ->START,STEP,STOP         *
C *                                     FORMAT (3F10.3)         *
C *                                          ON OFF             *
C *    PICK TYPE OF STATE TO OUTPUT : TYPE(1) -> GENERAL  1  0  *
C *                                   (2) -> RYDBERG    "       *
C *                                   (3) -> IONIZ.     "       *
C *                                                             *
C *    INPUT NUMBER OF STATES EACH TYPE AND PICK PARTICULAR STATES *
C *    TO OUTPUT:                                               *
C *          TYPE      NUM. OF STATES   PICK STATE              *
C *                                                             *
C *          GENERAL       NINEL          ISTATG                *
C *          RYDBERG       NRYD           ISTATR                *
C *          IONIZ.        NION           ISTATI                *
C *                                                             *
C *  IE. NINEL=5 AND ISTATE(1->5) = 2,3,4,6,8                   *
C *  WOULD PICK OUT GENERAL STATES 2,3,4,6,8 FOR OUTPUT         *
C *                                                             *
C *  SPECIAL SWITCH FOR MODIFIED VIBRATIONAL LEVELS ISWV=1      *
C *  ASSOCIATE KV = NUMBER OF VIBRATIONAL STATES WITH ISWV      *
C *                                                             *
C ***************************************************************
C
      READ(5,29) INEVEC
   29 FORMAT(I1)
C
      READ(5,20) (ITYPE(I),I=1,3)
   20 FORMAT(3I1)
C
      READ(5,21) NINEL,KV,NRYD,NION
   21 FORMAT(4I3)
C
      READ(5,22) (ISTATG(I),I=1,NINEL)
      READ(5,22) (ISTATR(I),I=1,NRYD)
      READ(5,22) (ISTATI(I),I=1,NION)
```

```
   22  FORMAT(3012)
C
       READ(5,23) ISWV,ISWR
   23  FORMAT(2I2)
C
C
C ****************************************************************
C
C INPUT ENERGY
       IF(INEVEC.NE.1) GOTO 121
       NE=0
  120  NE=NE+1
       READ(5,930) ISTP,E(NE)
       IF (ISTP.NE.1) GOTO 120
       GOTO 125
  121  READ(5,931) START,STEP,STOP
       NE=0
  122  NE=NE+1
       E(NE)=START
       START=START+STEP
       IF (START.LE.STOP) GOTO 122
  125  CONTINUE
  930  FORMAT (I1,F10.3)
  931  FORMAT (3F10.3)
C
C  ******************************************
C     INPUT TOTAL CROSS SECTION BELOW EIT(1)- APPROX. 20 EV
C
       READ(5,511)IEILS
  511  FORMAT(I2)
       IEILM1=IEILS-1
       READ(5,522)(EIT(MJ),MJ=1,IEILS)
       READ(5,522)(CSIE(MJ),MJ=1,IEILS)
  522  FORMAT(8E10.2)
C
       WRITE(6,520)
  520  FORMAT(/////,'1THE TOTAL INELASTIC CROSS SECTION IS READ IN FOR
     #ENERGIES BELOW 20 EV.  THE UNITS ARE 10**(-16) CM**2',//,
     #  4X,'ENERGY',6X,'CROSS SECTION',/)
C
       DO 26 MJ=1,IEILS
       WRITE(6,521)EIT(MJ),CSIE(MJ)
  521  FORMAT(2G15.7)
   26  CONTINUE
C
C*****************************************
C  INPUT PARAMETERS FOR STATES
C
C  GENERAL INELASTIC
C
```

```
C
      WRITE(6,623)
      WRITE(6,625)
C
      DO 7 KN=1,NINEL
        READ(5,524) GG1(KN),GG2(KN),GG3(KN),GG4(KN),WF(KN),WFA(KN),
     #  FACI(KN),ALFA(KN),BEFA(KN),CFA(KN),FFA(KN)
        IF (ISWV.EQ.1.AND.KN.LE.KV) READ(5,525) VIB1(KN),VIB2(KN),
     #  VIB3(KN)
        WRITE(6,627) GG1(KN),GG2(KN),GG3(KN),GG4(KN),WF(KN),ALFA(KN),
     #  BEFA(KN),WFA(KN),CFA(KN),FFA(KN),FACI(KN),VIB1(KN),VIB2(KN),
     #  VIB3(KN)
    7 CONTINUE
C
C  RYDBERG
C
C
       WRITE (6,711)
       WRITE(6,712)
C
      DO 8 KN=1,NRYD
        READ(5,710) GR1(KN),GR2(KN),GR3(KN),GR4(KN),RTHRI(KN),
     #  RALFA(KN),RBETA(KN),RDELTA(KN),RO(KN),RFF(KN),RTHR(KN)
        WRITE(6,713) GR1(KN),GR2(KN),GR3(KN),GR4(KN),RTHRI(KN),
     #  RALFA(KN),RBETA(KN),RDELTA(KN),RO(KN),RFF(KN),RTHR(KN)
  8   CONTINUE
C
      WRITE(6,629)
C
C  IGNIZATION
      DO 9 KN=1,NION
        READ(5,502) GI1(KN),GI2(KN),GI3(KN),GI4(KN),THRI(KN),
     #  (AKI(II,KN),II=1,2),(AJI(II,KN),II=1,3)
        READ(5,504)(GAMAI(II,KN),II=1,2),(TOI(II,KN),II=1,3)
        WRITE(6,611) GI1(KN),GI2(KN),GI3(KN),GI4(KN),THRI(KN),
     #  (AKI(II,KN),II=1,2),(AJI(II,KN),II=1,3),
     #  (GAMAI(II,KN),II=1,2),(TOI(II,KN),II=1,3)
C
  9   CONTINUE
C
C ************************************************************
C *                                                          *
C *    MAJOR DO LOOP OVER ENERGY TO CALCULATE INTEGRALS      *
C *                                                          *
C ************************************************************
C
      DO 1000 I=1,NE
C
        IF (ITYPE(1).EQ.0) GO TO 410
C
```

```
C    CALCULATE INTEGRALS FOR GENERAL
C
C
          DO 400 NJ=1,NINEL
            J=1
            K=ISTATG(NJ)
            IF(K.EQ.0) GO TO 400
            N=4
            Y(I,K,N,J)=FUN(0.0,E(I),0.0)
            TCSGEN(K,I)=TCSG
            CALL INT(I,E(I),Y,ER)
C-----------------------------------------------
C   SUM HI AND SOURCE
C   SUM HI AND SOURCE,  PUT IN HI POSITION
C   THEN DELETE SOURCE POSITION
       Y(I,K,1,J) = Y(I,K,1,J) + Y(I,K,4,J)
       Y(I,K,4,J) = 0.
C-----------------------------------------------
C
  400     CONTINUE
  410     CONTINUE
C
          IF (ITYPE(2).EQ.0) GO TO 510
C
C    CALCULATE INTEGRALS FOR RYDBERG
C
          DO 500 NJ=1,NRYD
            J=2
            K=ISTATR(NJ)
            IF(K.EQ.0) GO TO 500
            N=4
            Y(I,K,N,J)=FUN(0.0,E(I),0.0)
            TCSRYD(K,I)=TCSR
            CALL INT(I,E(I),Y,ER)
C-----------------------------------------------
C   SUM HI AND SOURCE
C   SUM HI AND SOURCE,  PUT IN HI POSITION
C   THEN DELETE SOURCE POSITION
       Y(I,K,1,J) = Y(I,K,1,J) + Y(I,K,4,J)
       Y(I,K,4,J) = 0.
C-----------------------------------------------
C
  500     CONTINUE
  510     CONTINUE
C
          IF (ITYPE(3).EQ.0) GO TO 610
C
C    CALCULATE INTEGRALS FOR IONIZATION
C
          DO 600 NJ=1,NION
```

```
          J=3
          K=ISTATI(NJ)
          IF(K.EQ.0) GO TO 600
          N=4
          Y(I,K,N,J)=FUN(0.0,E(I),0.0)
          TCSION(K,I)=TCSI
          CALL INT(I,E(I),Y,ER)
C-----------------------------------------------
C  SUM HI AND SOURCE
C  SUM HI AND SOURCE,  PUT IN HI POSITION
C  THEN DELETE SOURCE POSITION
      Y(I,K,1,J) = Y(I,K,1,J) + Y(I,K,4,J)
      Y(I,K,4,J) = 0.
C-----------------------------------------------
C
  600   CONTINUE
  610   CONTINUE
C
C
1000  CONTINUE
C
C ****************************************************************
C *                                                              *
C *     WRITE OUT THE STATES AND THEIR INTEGRATED YIELDS         *
C *                                                              *
C ****************************************************************
C
      DO 899 I=1,NE
C
         WRITE(6,820)
         WRITE(6,800) E(I)
         WRITE(6,801)
C
      IF (ITYPE(I).EQ.0) GO TO 819
C
C
         DO 818 KN=1,NINEL
           KG=ISTATG(KN)
           IF (KG.EQ.0) GO TO 818
C
      YSUM=(Y(I,KG,1,1)+Y(I,KG,2,1)+Y(I,KG,3,1)+Y(I,KG,4,1))/E(I)
C
         WRITE(6,811) GG1(KG),GG2(KG),GG3(KG),GG4(KG),KG,
     #   TCSGEN(KG,I),Y(I,KG,4,I),(Y(I,KG,JJ,1),ER(I,KG,JJ,1),JJ=1,3)
     #   ,YSUM
      IF (ISWR.EQ.1) WRITE(9,812) E(I),KG,(Y(I,KG,JJ,1),JJ=1,4)
  818   CONTINUE
C
  819   CONTINUE
C
```

```
      IF (ITYPE(2).EQ.0) GO TO 829
C
        WRITE(6,820)
C
        DO 828 KN=1,NRYD
          KR=ISTATR(KN)
          IF (KR.EQ.0) GO TO 828
C
      YSUM=(Y(I,KR,1,2)+Y(I,KR,2,2)+Y(I,KR,3,2)+Y(I,KR,4,2))/E(I)
C
        WRITE(6,811) GR1(KR),GR2(KR),GR3(KR),GR4(KR),KR,
     #    TCSRYD(KR,I),Y(I,KR,4,2),(Y(I,KR,JJ,2),
     #    ER(I,KR,JJ,2),JJ=1,3),YSUM
      IF (ISWR.EQ.1) WRITE(9,812) E(I),KR,(Y(I,KR,JJ,2),JJ=1,4)
  828   CONTINUE
C
  829   CONTINUE
C
      IF (ITYPE(3).EQ.0) GO TO 840
C
        WRITE(6,820)
C
        DO 839 KN=1,NION
          KI=ISTATI(KN)
          IF (KI.EQ.0) GO TO 839
C
      YSUM=(Y(I,KI,1,3)+Y(I,KI,2,3)+Y(I,KI,3,3)+Y(I,KI,4,3))/E(I)
C
        WRITE(6,811) GI1(KI),GI2(KI),GI3(KI),GI4(KI),KI,
     #    TCSION(KI,I),
     #    Y(I,KI,4,3),(Y(I,KI,JJ,3),ER(I,KI,JJ,3),JJ=1,3),YSUM
      IF (ISWR.EQ.1) WRITE(9,812) E(I),KI,(Y(I,KI,JJ,3),JJ=1,4)
  839   CONTINUE
C WRITE OUT TOTALS
C
  840   CONTINUE
C
  899 CONTINUE
C
C ***********************READ/WRITE FORMAT STATEMENTS******************
C
 623  FORMAT(' ',//,' THE STATES WITH THEIR CROSS SECTION PARAMETERS ARE
     #READ IN',//)
 625  FORMAT(' ',6X,'STATE',11X,'W',7X,'ALPHA',4X,'BETA',6X,
     #  'WBAR',7X,'C OR G',10X,'F',6X,'FACI',9X,'VIB1',
     # 7X,'VIB2',7X,'VIB3',/)
 524  FORMAT(4A4,4X,6E6.0,E11.4)
 525  FORMAT(3E11.4)
 627  FORMAT(' ',1X,4A4,3F9.3,F10.3,F11.3,F15.6,5E11.4)
 710  FORMAT(4A4,4X,7E6.0)
```

```
 711  FORMAT(' ',//,' RYDBERG STATES',/)
 712  FORMAT(' ',6X,'STATE',9X,'THRI',5X,'ALPHA',4X,'BETA',6X,'DELTA',
     # 6X,'C OR O',10X, 'F* ',7X,'THR',/)
 713  FORMAT(' ',1X,4A4,3F9.3,F10.3,F11.3,F15.6,F9.3)
 629  FORMAT(' ',///' THE S(E,T) PARAMETERS FOLLOW',//,4X,'ION. STATES',
     #6X,'THRI',6X,'KI',6X,'KBI',5X,'JI',5X,'JBI',5X,'JCI',6X,
     #'GAMSI',4X,'GAMBI',6X,'TSI',6X,'TAI',4X,'TBI',/)
 502  FORMAT(4A4,4X,7E8.0)
 504  FORMAT(20X,5E8.0)
 611  FORMAT(' ',1X,4A4,F8.3,1X,5F8.3,2X,2F8.3,F10.3,F8.1,F8.3)
 800  FORMAT(' ',/,130('*'),/,' AT THE ENERGY ',F8.3,' THE ',
     #  ,' CROSS SECTIONS SIGMA(E) AND INTEGRATED YIELDS  ARE:')
 801  FORMAT(' ',/,T3,'STATE',T20,'NUM.',T29,'CROSS SECTION',T50,
     #  'P(E)',T70,'YIELDS AND %ERROR: 1->3 ',23X,' TOT. YIELD/EV')
C
C
 811  FORMAT(' ',1X,4A4,1X,I2,6X,G10.3,5X,G10.3,2X
     #,3(G10.3,1X,G9.2,'%',1X),G10.3)
 812  FORMAT(' ',F8.2,2X,I3,1X,4(1X,E14.7))
 820  FORMAT(/)
C
C
C
C
      STOP
      END
-------------------------------
-------------------------------
          YIELD.B
-------------------------------
      SUBROUTINE INT(I,EV,Y,ER)
C
      EXTERNAL FUN
C
      DIMENSION RALFA(4),RTHRI(4),RBETA(4),RO(4),RFF(4),RDELTA(4)
      DIMENSION RTHR(4)
      DIMENSION THRI(6),AKI(2,6),AJI(3,6),TOI(3,6),GAMAI(2,6)
      DIMENSION WF(23),WFA(23),FACI(23),ALFA(23),BEFA(23),CFA(23),
     #FFA(23),VIB1(23),VIB2(23),VIB3(23)
      DIMENSION Y(20,30,4,3),ER(20,30,4,3)
C
      COMMON/CONST/  Q0
      COMMON/PARAG/ WF,WFA,FACI,ALFA,BEFA,CFA,FFA,VIB1,VIB2,VIB3
     #,ISWV,KV
      COMMON/PARAR/ RTHRI,RALFA,RBETA,RO,RDELTA,RFF,RTHR
      COMMON/PARAI/ THRI,AKI,AJI,GAMAI,TOI
      COMMON/FUNSW/ K,N,J,EK
C
      EK=EV/1000.
C
```

:

```
      DO 1000 N=1,3
C
      TOL=1.0
      PERR=.1
C
      DO 500 M=1,3
C
      GO TO (100,200,300),J
C
 100  A=VM1D(TOL,WFA(K),EV,FUN,ERRE,0,10,256)
C     WRITE(6,333) TOL,J,WFA(K),EV,N,M,A
C 333  FORMAT(' ',7G14.7)
C
      GO TO 400
 200  A=VM1D(TOL,RTHRI(K),EV,FUN,ERRE,0,10,256)
C     WRITE(6,333) TOL,J,RTHRI(K),EV,N,M,A
      GO TO 400
 300  A=VM1D(TOL,THRI(K),EV,FUN,ERRE,0,10,256)
C     WRITE(6,333) TOL,J,THRI(K),EV,N,M,A
      GO TO 400
 400  CONTINUE
      APERR=ERRE
      IF (A.GT.1.0E-50) APERR=100.*ERRE/A
      TOL=AMAX1(.03*A,.3*ERRE)
      IF (APERR.LT.PERR) GO TO 510
 500  CONTINUE
 510  CONTINUE
C
      Y(I,K,N,J)=A
      ER(I,K,N,J)=APERR
 1000 CONTINUE
C
      RETURN
      END
      FUNCTION FUN(TLF,X,ERF)
C
      DIMENSION RALFA(4),RTHRI(4),RBETA(4),RO(4),RFF(4),RDELTA(4)
      DIMENSION RTHR(4)
      DIMENSION THRI(6),AKI(2,6),AJI(3,6),TOI(3,6),GAMAI(2,6)
      DIMENSION WF(23),WFA(23),FACI(23),ALFA(23),BEFA(23),CFA(23),
     #FFA(23),VIB1(23),VIB2(23),VIB3(23)
      DIMENSION EIT(60),CSIE(60)
C
      COMMON/CONST/  Q0
      COMMON/PARAG/ WF,WFA,FACI,ALFA,BEFA,CFA,FFA,VIB1,VIB2,VIB3
     #,ISWV,KV
      COMMON/PARAR/ RTHRI,RALFA,RBETA,RO,RDELTA,RFF,RTHR
      COMMON/PARAI/ THRI,AKI,AJI,GAMAI,TOI
      COMMON/FUNTCS/ EIT,CSIE,TCSG,TCSR,TCSI,IEILM1
      COMMON/FUNSW/ K,N,J,EK
```

```
C
      ERF=1.0E-07
C
C   CALCULATE TCST THE TOTAL INELASTIC CROSS SECTION.
C
      IF(X .LT. EIT(1))GO TO 1
C
      ST1=ALOG(.022*(X/5.534-1.)**1.774+1.)
      ST2=1.774*5.534*X
      TCST=Q0*2.962*ST1/ST2
      GO TO 4
    1 CONTINUE
      KK=0
      DO 2 JK=1,IEILM1
      KK=KK+1
      KKP1=KK+1
      IF(X .LE. EIT(KK) .AND. X .GE. EIT(KKP1))GO TO 3
    2 CONTINUE
    3 TCST=CSIE(KK)+(X-EIT(KK))*(CSIE(KKP1)-CSIE(KK))
     #/(EIT(KKP1)-EIT(KK))
      IF (X.LT.WFA(1)) TCST=0.0
    4 CONTINUE
C
      GO TO (100,200,300),J
C
  100 CONTINUE
        IF(X.LT.WFA(K)) GO TO 390
        TEMP=WF(K)/X
        IF (TEMP.GT.1.) TEMP=1.
        ST1=(1.-TEMP**ALFA(K))**BEFA(K)
        ST2=TEMP**CFA(K)
        TCSG=Q0*ST1*ST2*(FFA(K)/(WF(K)*WF(K)))
        IF (ISWV.EQ.1.AND.K.LE.KV) TCSG=TCSG + VIB1(K)/
     #  ((VIB3(K)-X)*(VIB3(K)-X)+VIB2(K))
C       WRITE(6,334) K,N,J,X,TCST,WF(K),WFA(K),TCSG,ISWV,KV
C 334  FORMAT(' ',10G12.5)
        PP=TCSG/TCST
      GO TO 400
  200 CONTINUE
C
        IF(X.LT.RTHRI(K))GO TO 390
C
        TOTRYD=0.0
C
        DO 262 NN=3,3
          IF(NN.EQ.3) GO TO 260
          W=RTHR(K)-(13.6/((NN-RDELTA(K))**2))
          F=RFF(K)/((NN/RDELTA(K))**3)
          GO TO 261
  260     CONTINUE
```

```
C   PARTICULAR VALUE FOR WATER VAPOR
          W=RTHR(K)-(13.6/((NN-RDELTA(K))**2))
          F=RFF(K)/((2*(NN-RDELTA(K)-.5))**2)
  261     CONTINUE
          TEMP=W/X
          IF (TEMP.GT.1.) TEMP=1.0
          ST1=(1.-TEMP**RALFA(K))**RBETA(K)
          ST2=TEMP**RQ(K)
          SIGRN=Q0*ST1*ST2*(F/(W*W))
          SUBRYD=SIGR+SIGRN
          TOTRYD=TOTRYD+SUBRYD
  262     CONTINUE
        TCSR=TOTRYD
        PP=TCSR/TCST
      GO TO 400
C
 300  CONTINUE
C
        IF(X.LT. THRI(K)) GO TO 390
C
        TSET=TOI(1,K)-TOI(2,K)/(X+TOI(3,K))
        GSET=GAMAI(1,K)*X/(X+GAMAI(2,K))
        TM=(X-THRI(K))/2.
        ASET=(AKI(1,K)/(X+AKI(2,K)))*ALOG(X/AJI(1,K)+
     #  AJI(2,K)+AJI(3,K)/X)
        TCSI=ASET*GSET*(ATAN((TM-TSET)/GSET)+
     #  ATAN(TSET/GSET))
        PP=TCSI/TCST
      GO TO 400
C
 390  CONTINUE
C
      FUN=0.0
      RETURN
C
 400  CONTINUE
C
      U2 = .0282 + 902.*EK/(X*X + 3.21*3.21)
C          DATA EPS, BBB, PPP, AAA/ .197, 2.65E-5, 1.75, 1.34E7 /
C  AAA NOT USED, CANCELS OUT IN RATIO
      EPS = .197
      BBB = 2.65E-5
      PPP = 1.75
      AAA = 1.34E7
      E0 = 1000.*EK
      F = (X**EPS + BBB*X**PPP)/(E0**EPS + BBB*E0**PPP)
C
      GO TO (500,600,700,800),N
C
 500  CONTINUE
```

```
      FUN = PP*F*U2
      RETURN
600   CONTINUE
      FUN = PP*(1. - F)*U2
      RETURN
700   CONTINUE
      FUN=0.0
      RETURN
800   CONTINUE
      FUN=PP
      RETURN
      END
```

BIBLIOGRAPHY

Allis, W. P., 1956. In Handbuch der Physik, ed. S. Flugge, Berlin: Springer-Verlag, pp. 383-444.

Bethe, H. A. 1932. Z. Physik, 76:293.

Birkhoff, G., and G.-C. Rota. 1962. Ordinary Differential Equations, Waltham, Massachusetts: Blaisdell Publ. Co.

Brenner, D. J. 1982. A Computationally Convenient Parameterization of Experimental Angular Distributions of Low Energy Electrons Elastically Scattered Off Water Vapor, Los Alamos, New Mexico: Los Alamos National Lab.

Brenner, D. J., and M. Zaider. 1983. In proceedings, Workshop on the Interface between Radiation Chemistry and Radiation Physics, pp. 58-64, Argonne National Laboratory, Prepared for U.S. Dept. of Energy, Contract W-31-109-Eng-38, Argonne, Illinois, Argonne National Laboratory.

Brown, S. C. 1958. In Handbook of Physics, ed. E. U. Condon and H. Odishaw, New York: Mc-Graw-Hill Book Co. 4:159-

Brown, S. C., and W. P. Allis. 1963. In American Institute of Physics Handbook, ed. D. E. Gray, New York: McGraw-Hill Book Co. 7:184-229.

Burden, R. L., J. D. Faires, and A. C. Reynolds. 1978. Numerical Analysis, Prindle, Weber and Schmidt, Boston.

Chatterjee, A. and J. L. Magee. 1980. J. Phys. Chem. 84:3537-3543.

Christophorou, L. G. ed. 1981. Electron and Ion Swarms, New York: Pergamon Press.

Coldwell, R. L. 1979. Private communication.

Dahlquist, G., and A. Bjorck, 1974. Numerical Methods, Englewood Cliffs, New Jersey: Prentice-Hall, Inc.

Dash, S. M., and H. S. Pergament. 1978. NASA Contractor Report 3075: A Computational Model for the Prediction of Jet Entrainment in the Vicinity of Nozzle Boattails [The BOAT Code].

Douthat, D. A. 1983. In proceedings, Workshop on the Interface between Radiation Chemistry and Radiation Physics, pp. 134-136. Prepared for U.S. Dept. of Energy, Contract W-31-109-Eng-38, Argonne, Illinois: Argonne National Laboratory.

Dwight, H. B. 1961. Table of Integrals and Other Mathematical Data, New York: Macmillan Publ. Co.

Eisberg, R. M. 1961. Fundamentals of Modern Physics, New York: John Wiley and Sons, Inc.

Ferguson, E. E. 1973. Atom. Data Nucl. Data Tables 12:159.

Flanders, D. A., and H. Fricke. 1958. J. Chem. Phys. 28:1126.

Good, A., D. A. Durden, and P. Kerbarle. 1970. J. Chem. Phys. 52:212.

Green, A. E. S. 1955. Nuclear Physics, New York: McGraw-Hill Book Co.

Green, A. E. S. 1984. Private communication.

Green, A. E. S., and C. A. Barth. 1965. J. Geophys. Res., 70:1083.

Green, A. E. S., and J. Burki. 1974. Rad. Res., 60:536-540.

Green, A. E. S., and S. K. Dutta. 1967. J. Geophys. Res. 72:3933-3941.

Green, A. E. S., R. H. Garvey, and C. H. Jackman. 1977. Int. J. Quantum Chem. Symp. 11:97-103.

Green, A. E. S., C. H. Jackman, and R. H. Garvey. 1977. J. Geophys. Res. 82:5104.

Green, A. E. S., J. J. Olivero, and R. W. Stagat. 1971. Biophysical Aspects of Radiation Quality. Vienna: Int. Atomic Energy Agency.

Green, A. E. S., and R. R. Singhal. 1979. Geophys. Res. Letters 6:625-628.

Green, A. E. S., and R. S. Stolarski. 1972. J. Atmosph. Terr. Phys. 34:1703-1717.

Grün, Von A. E. 1957. Z. Naturforsch. 12a:89-95.

Hamm, R. N., H. A. Wright, J. E. Turner, and R. H. Ritchie. 1978. In proceedings, 6th Symposium on Microdosimetry (Brussels, Belgium), ed. J. Booz and H. G. Ebert, p. 179. Commission of the European Communities, EUR-6064-DE-EN-FR. London: Harwood Academic Pub.

Hamm, R. N., R. H. Ritchie, J. E. Turner, and H. A. Wright. 1983. In proceedings, Workshop on the Interface between Radiation Chemistry and Radiation Physics, pp. 32-36. Prepared for U. S. Dept. of Energy, Contract W-31-109-Eng-38. Argonne, Illinois: Argonne National Laboratory.

Hanrahan, R. J. 1983. In proceedings, Workshop on the Interface between Radiation Chemistry and Radiation Physics, pp. 132-133. Prepared for U. S. Dept. of Energy, Contract W-31-109-Eng-38. Argonne, Illinois: Argonne National Laboratory.

Hart, E. J. and R. L. Platzmann. 1961. In Mechanisms in Radiobiology, ed., A. Hollaender, Vol. I, Chap. 2, New York: Academic Press.

Hindmarsh, A. C. 1974. GEAR: ordinary differential equation system solver, Report UCID 30001, Rev. 3, December. Oakland: Lawrence Livermore Laboratory.

Hirschfelder, J. O., C. F. Curtiss, and R. B. Bird. 1954. Molecular Theory of Gases and Liquids. New York: Wiley and Sons.

Huntress, W. T. 1973. Astrophy. J. Suppl. Ser. 33:495.

IMSL Library Edition 8. 1981. Houston, Texas: International Mathematical Subroutine Library, Inc.

Inokuti, M. 1983. In proceedings, Workshop on the Interface between Radiation Chemistry and Radiation Physics, pp. 4-8. Prepared for U. S. Dept. of Energy, Contract W-31-109-Eng-38. Argonne, Illinois: Argonne National Laboratory.

Jackman, C. H. 1978. Spatial and Energetic Aspects of Electron Energy Deposition. Ph. D. dissertation, University of Florida, Gainesville.

Jackman, C. H., and A. E. S. Green. 1979. Geophys. Res. 84:2715.

Jackman, C. H., R. H. Garvey, and A. E. S. Green. 1977. J. Geophys. Res. 82:5081-5090.

Jackson, J. D. 1967. Classical Electrodynamics, New York: J. Wiley and Sons, Inc.

Katz, L., and A. S. Penfold. 1952. Revs. Mod. Phys., 24:30- .

Kee, R. J., and J. A. Miller. 1978. AIAA Journal, 16:2:169-176.

Kee, R. J., J. Warnatz, and J. A. Miller. 1983. A Fortran Computer Code Package for the Evaluation of Gas-Phase Viscosities, Conductivities and Diffusion Coefficients, Sandia Report, Sand. 83-8209, Contract DE-AC04-76DP00789, Albuquerque, New Mexico and Livermore, California: Sandia National Laboratory.

Kupperman, A. 1974. Physical Mechanisms in Radiation Biology. ed. R. D. Cooper and R. W. Wood, 155-176. Conf. 721001. Washington: Tech. Info. Ctr., Ofc. Info. Services.

Kupperman, A., and G. G. Belford. 1962a. J. Chem. Phys. 36:1412-1426.

Kupperman, A., and G. G. Belford. 1962b. J. Chem. Phys. 36:1427-1441.

Kutcher, G. J., and A. E. S. Green. 1976a. Rad. Res. 67:408-425.

Kutcher, G. J., and A. E. S. Green. 1976b. J. Applied Physics 47:2175-2183.

Lea, D. E. 1946. Actions of Radiations on Living Cells, New York: Cambridge University Press.

Lea, D. E. 1947. British J. Radiol. Suppl. 1:59.

Leu, M. T., M. A. Biondi, and R. Johnsen. 1973. Phys. Rev. 8:413.

Magee, J. L. 1963. Discussions Faraday Soc., 36:116, 232.

Magee, J. L., and A. Chatterjee. 1978. J. Phys. Chem. 82:2219-2226.

Magee, J. L., and A. Chatterjee. 1980. J. Phys. Chem. 84:3529-3536.

Magee, J. L., and A. Chatterjee. 1983a. In proceedings, Workshop on the Interface between Radiation Chemistry and Radiation Physics, pp. 121-122, Argonne National Laboratory, Prepared for U. S. Dept. of Energy, Contract W-31-109-Eng-38, Argonne, Illinois, Argonne National Laboratory.

Magee, J. L., and A. Chatterjee. 1983b. In proceedings, Workshop on the Interface between Radiation Chemistry and Radiation Physics, pp. 126-127, Argonne National Laboratory, Prepared for U. S. Dept. of Energy, Contract W-31-109-Eng-38, Argonne, Illinois, Argonne National Laboratory.

Miller, J. A., and R. J. Kee. 1977. J. Phys. Chem. 81:2534-2542.

Monchick, L., and E. A. Mason. 1961. J. Chem. Phys. 35:1676.

Monchick, L., J. L. Magee, and A. H. Samuel. 1957. J. Chem. Phys. 26:935-941.

Mooney, J. R. 1984. SIAM J. Appl. Math. 44:4, 745-761.

Morse, P. M., and H. Feshbach. 1953. Methods of Theoretical Physics, New York: McGraw-Hill Book Co.

Olivero, J. J., R. W. Stagat, and A. E. S. Green. 1972. J. Geophys. Res. 17:4797-4811.

Pamidimukkala, K. M., P. F. Schippnick, D. B. Vaidya, and A. E. S. Green. 1983. In Proceedings of the 15th Annual JANNAF Plume Technology Meeting, China Lake, California.

Peterson, L. R. 1969. Phys. Rev. 187:105-111.

Porter, H. S., and F. W. Jump. 1978. Report CSC/TM-78/6017. Prepared by Computer Science Corp. for Goddard Space Flight Ctr., Washington, D. C.

Reif, F. 1965. Fundamentals of Statistical and Thermal Physics, New York: McGraw-Hill Book Co.

Rio, D. E. 1983. Private communication.

Rio, D. E. 1983. A Study of the Effects of Diffusion and Kinetics on the Spatial Distribution of Products Created by Electron Deposition, Ph.D. Dissertation, University of Florida.

Rio, D. E., Dayashankar, P. F. Schippnick, and A. E. S. Green, in preparation.

Ritchie, R. H., R. N. Hamm, J. E. Turner, and T. P. Turner. 1978. In proceedings, 6th Symposium on Microdosimetry (Brussels, Belgium), ed. J. Booz and H. G. Ebert, pp. 345-354. Commission of the European Communities, EUR-6064-DE-EN-FR. London: Harwood Academic Publ.

Samuel, A. H., and J. L. Magee. 1953. J. Chem. Phys. 21:1080.

Seng, G. 1975. Das System (e-H_2O) Differentielle Streuexperiment bei Kleinsten Energien. Thesis, Kaiserslautern Univ., Kaiserslautern, West Germany.

Singhal, R. P., and A. E. S. Green. 1981. J. of Geophys. Res. 86(A6):4776-4780.

Singhal, R. P., C. H. Jackman, and A. E. S. Green. 1980. J. of Geophys. Res. 85(A3):1246-1254.

Singhal, R. P., D. E. Rio, P. F. Schippnick, and A. E. S. Green. 1983. Rad. Res. 95:32-44.

Spencer, L. V., and V. Fano. 1954. Physical Review 93:1172-1181.

Stolarski, R. S., and A. E. S. Green. 1967. J. Geophys. Res. 72:3967-3974.

Turner, J. E., H. G. Paretzke, R. N. Hamm, H. A. Wright, and R. H. Ritchie. 1983. In proceedings, Workshop on the Interface between Radiation Chemistry and Radiation Physics, pp. 91-100. Prepared for U. S. Dept. of Energy, Contract W-31-109-Eng-38. Argonne, Illinois: Argonne National Laboratory.

TWODEPEP Edition 3. 1981. Houston, Texas: International Mathematical Subroutine Library, Inc.

Verhulst, P. F. 1838. Corresp. Math. Phys., 10:113-121.

Westbrook, C. K. 1981. Hydrogen Oxidation Kinetics in Gaseous Detonations, Combustion Science and Technology, rev. 1.

Wright, H. A., J. E. Turner, R. N. Hamm, R. H. Ritchie, J. L. Magee, and A. Chatterjee. 1983a. In proceedings, Eighth Symposium on Microdosimetry (Julich, West Germany), in press.

Wright, H. A., J. E. Turner, R. N. Hamm, R. H. Ritchie, J. L. Magee, and A. Chatterjee. 1983b. In proceedings, Workshop on the Interface between Radiation Chemistry and Radiation Physics, pp. 106-112. Prepared for U. S. Contract W-31-109-Eng-38. Argonne, Illinois: Argonne National Laboratory.

Zaider, M., and D. J. Brenner. 1983. In proceedings, Workshop on the Interface between Radiation Chemistry and Radiation Physics, pp. 113-120. Prepared for U. S. Dept. of Energy, Contract W-31-109-Eng-38. Argonne, Illinois: Argonne National Laboratory.

BIOGRAPHICAL SKETCH

Paul Frederick Schippnick was born in Miami, Florida, on December 26, 1947. His father was born and raised in New York State, and worked for forty years for F. W. Dodge Corporation in construction news. His mother was born in Vienna, Austria, and grew up there and in Czechoslovakia before emigrating to this country November, 1938 and becoming an American citizen. He has one sister, Candace, three years younger.

The author graduated from Chamberlain High School in Tampa, Florida, in June of 1965, thirteenth in a class of 772. He then entered the University of Florida as a freshman in 1965, and received the degree of Bachelor of Science in physics with honors and was inducted into Phi Beta Kappa in 1969. He then entered the University of California, San Diego, where he completed requirements for the degree of Master of Science in physics in 1972 and received it in 1974 upon application. From early 1976 through early 1979 he was employed by Chapman College, Orange, California, as instructor in mathematics aboard various ships in the 7th Fleet of the U. S. Navy and in port in San Diego, in the Program of Afloat College Education (PACE). In June of 1979 the author recommenced his graduate studies under the tutelage of Prof. Alex E. S. Green, for whom he had worked as a student assistant in 1968 and 1969.

On September 15, 1982 the author married Dr. Aleksandra Nowacka, who was attending the University of Florida as an International Exchange Scholar from the University of Warsaw, Poland. On June 29, 1984, a daughter, Sophia Theresa, was born to them.

I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.

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December 1984

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Dean for Graduate Studies
and Research